Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (neutral XH) 3.05 ±0.01 (n=50)
logP (X -) -0.40 ±0.05 (n=50)

18C-02007 Points 2 to 38

M08_octanol concentration factor 1.137
Carbonate 0.0754 mM
Acidity error -1.80478 mM

18C-02007 Points 39 to 77

M08_octanol concentration factor 0.855
Carbonate 0.3938 mM
Acidity error -1.60863 mM

18C-02007 Points 78 to 114

M08_octanol concentration factor 0.850
Carbonate 0.3937 mM
Acidity error -1.48346 mM

Warnings and errors

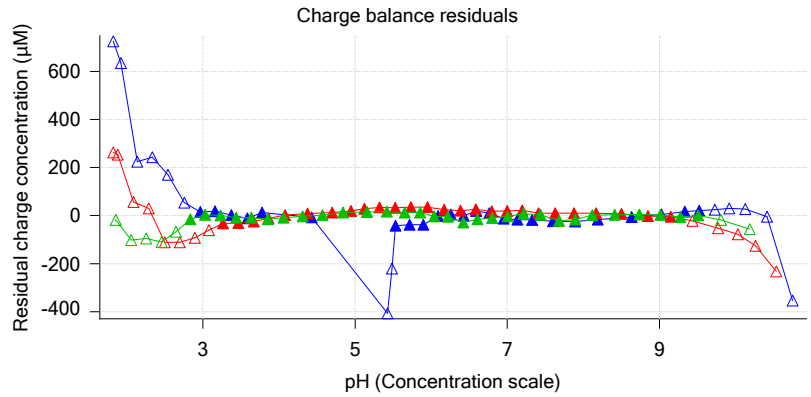
Errors None
Warnings None

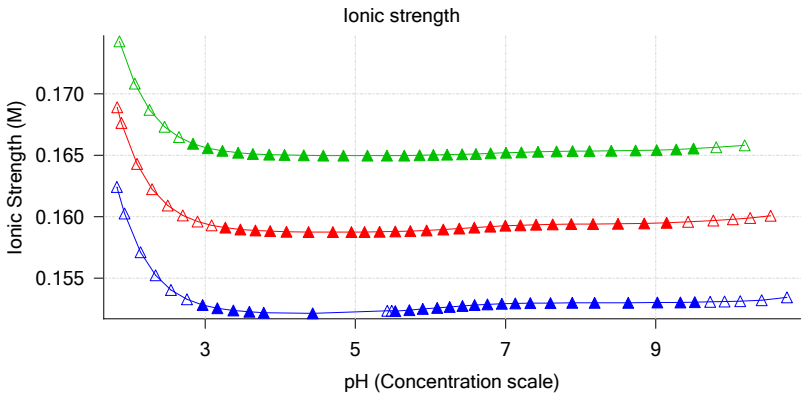
Sample logD and percent species

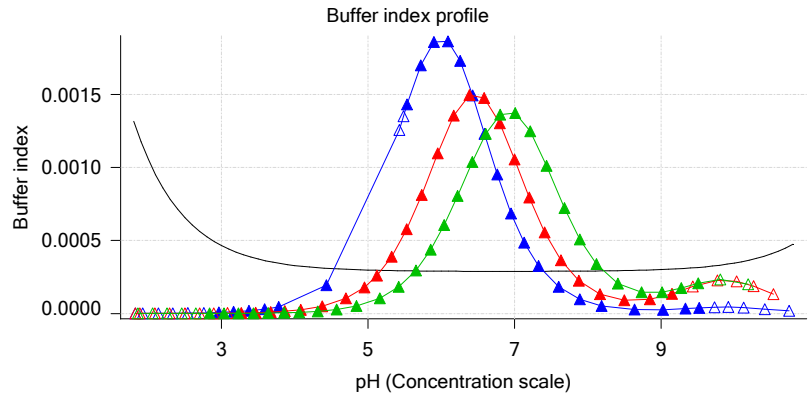
pH	M08_octanol logD	M08_octanolH	M08_octanol	M08_octanolH*	M08_octanol*	Comment
1.000	3.05	0.09 %	0.00 %	99.91 %	0.00 %	
1.200	3.05	0.09 %	0.00 %	99.91 %	0.00 %	Stomach pH
2.000	3.05	0.09 %	0.00 %	99.91 %	0.00 %	
3.000	3.03	0.09 %	0.01 %	99.90 %	0.00 %	
4.000	2.85	0.09 %	0.05 %	99.84 %	0.02 %	
5.000	2.21	0.09 %	0.53 %	99.18 %	0.21 %	
6.000	1.28	0.08 %	4.94 %	93.03 %	1.95 %	
6.500	0.80	0.07 %	13.61 %	80.97 %	5.36 %	
7.000	0.36	0.05 %	30.52 %	57.42 %	12.01 %	
7.400	0.06	0.03 %	46.65 %	34.95 %	18.36 %	Blood pH
8.000	-0.24	0.01 %	63.21 %	11.90 %	24.88 %	
9.000	-0.38	0.00 %	70.80 %	1.33 %	27.87 %	
10.000	-0.40	0.00 %	71.66 %	0.13 %	28.21 %	
11.000	-0.40	0.00 %	71.74 %	0.01 %	28.24 %	
12.000	-0.40	0.00 %	71.75 %	0.00 %	28.25 %	

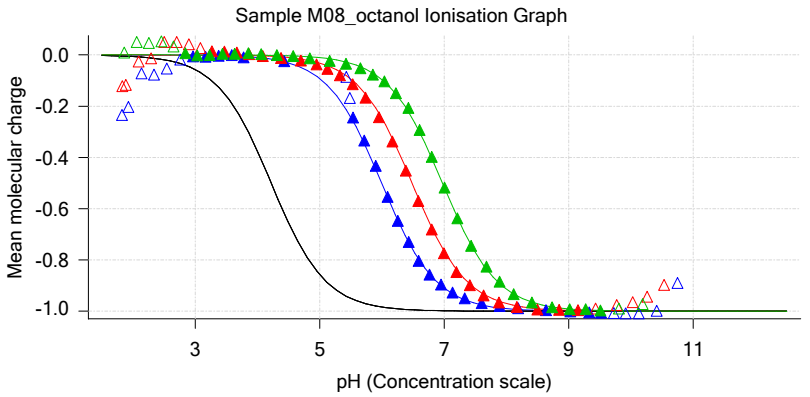
Sample name:	**M08_octanol**	Experiment start time:	**3/2/2018 5:10:52 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-02007**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**		

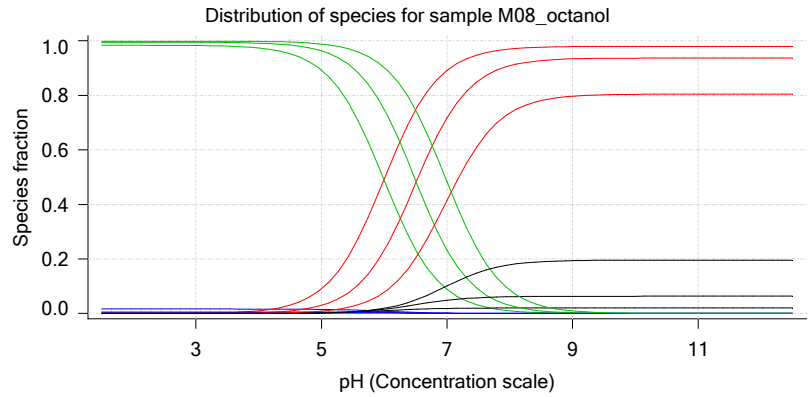
Graphs

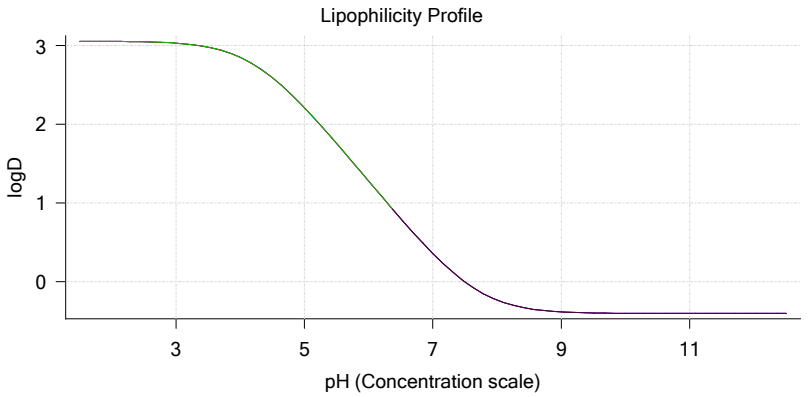


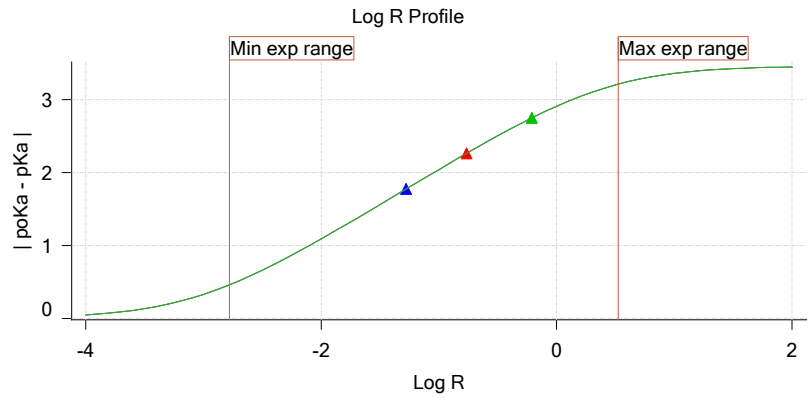


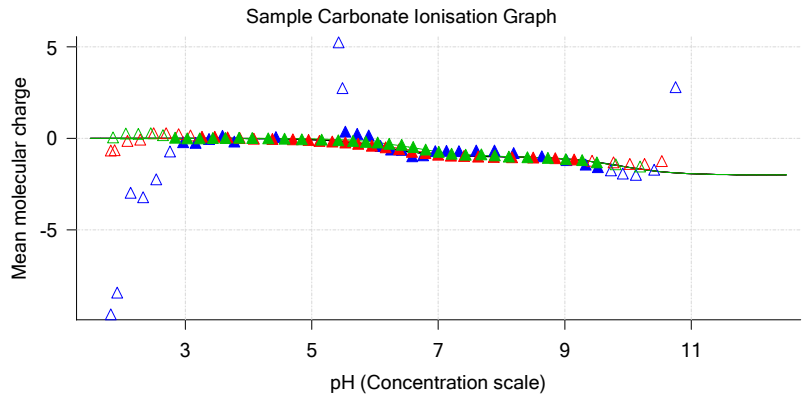








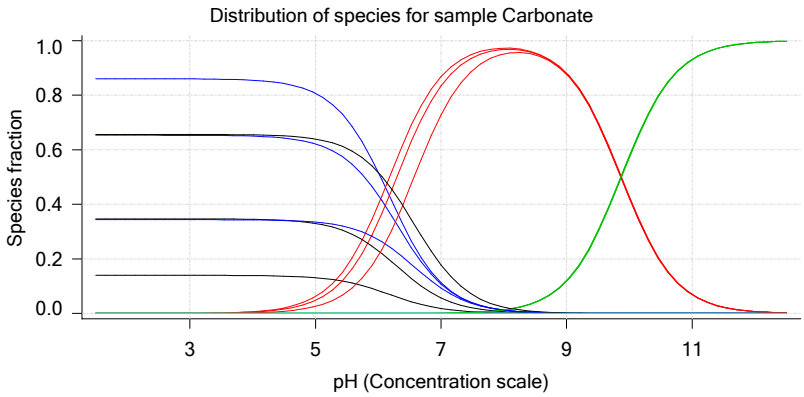




Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M08_octanol**	Experiment start time:	**3/2/2018 5:10:52 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-02007**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18C-02007 Points 2 to 38

Overall results

RMSD	0.092
Average ionic strength	0.153 M
Average temperature	25.0°C
Partition ratio	0.0526 : 1
Analyte concentration range	2593.3 µM to 2686.2 µM
Total points considered	24 of 37

Warnings and errors

Errors	None
Warnings	One or more logP values out of range
	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r

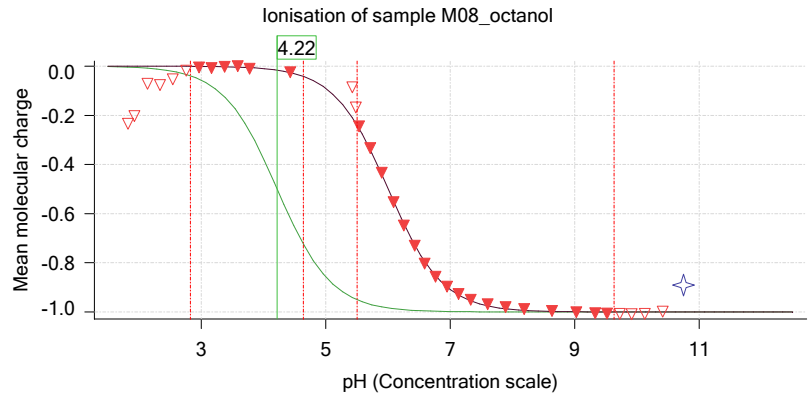
Titrants

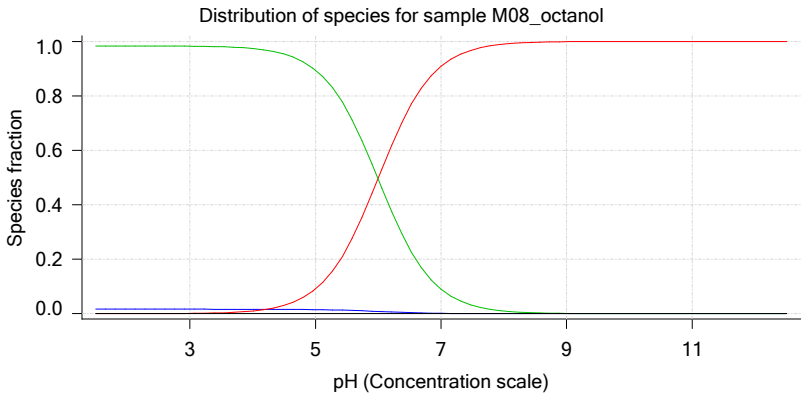
0.50 M HCl	0.999058	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 5:10:52 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor	1.137
Acid pKa 1	4.22
logP (neutral XH)	3.06
logP (X -)	-5.22

Sample graphs

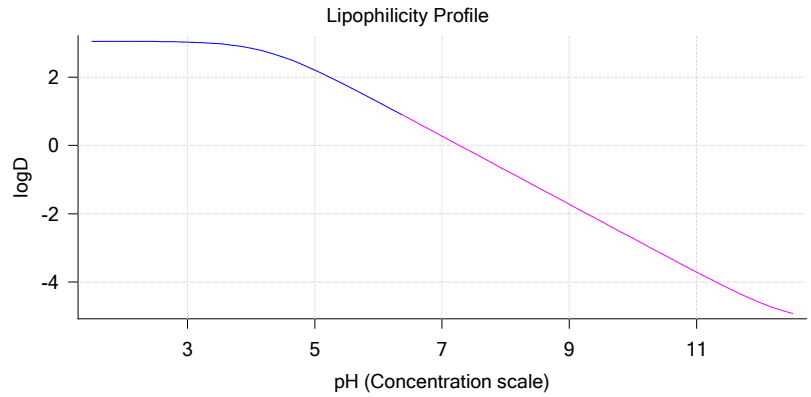




Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



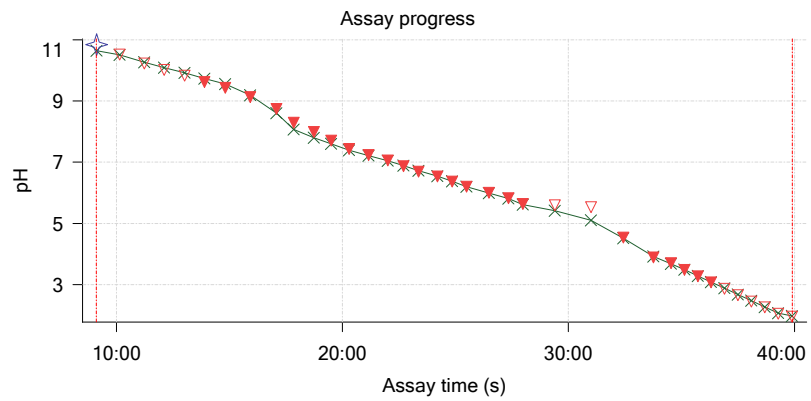
Sample logD and percent species

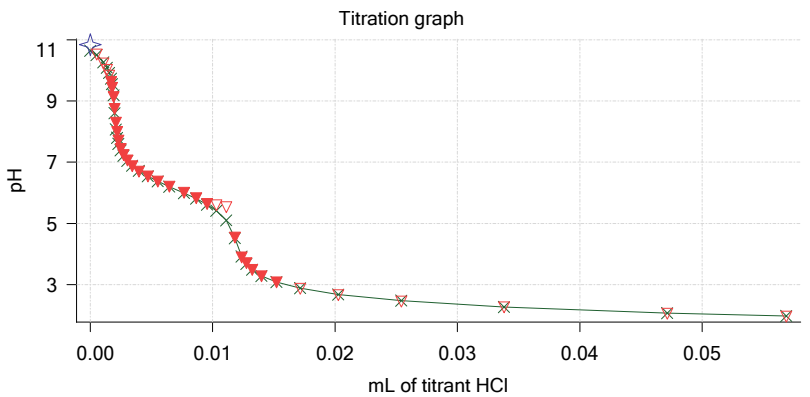
pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.05	1.65 %	0.00 %	98.35 %	0.00 %	
1.200	3.05	1.65 %	0.00 %	98.35 %	0.00 %	Stomach pH
2.000	3.05	1.65 %	0.01 %	98.34 %	0.00 %	
3.000	3.03	1.65 %	0.10 %	98.26 %	0.00 %	
4.000	2.85	1.63 %	0.98 %	97.39 %	0.00 %	
5.000	2.21	1.50 %	9.03 %	89.48 %	0.00 %	
6.000	1.27	0.83 %	49.80 %	49.37 %	0.00 %	
6.500	0.77	0.40 %	75.83 %	23.77 %	0.00 %	
7.000	0.27	0.15 %	90.84 %	9.00 %	0.00 %	
7.400	-0.13	0.06 %	96.14 %	3.79 %	0.00 %	Blood pH
8.000	-0.72	0.02 %	99.00 %	0.98 %	0.00 %	
9.000	-1.72	0.00 %	99.90 %	0.10 %	0.00 %	
10.000	-2.72	0.00 %	99.99 %	0.01 %	0.00 %	
11.000	-3.71	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.60	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.075 mM
Acidity error -1.805 mM

Other graphs

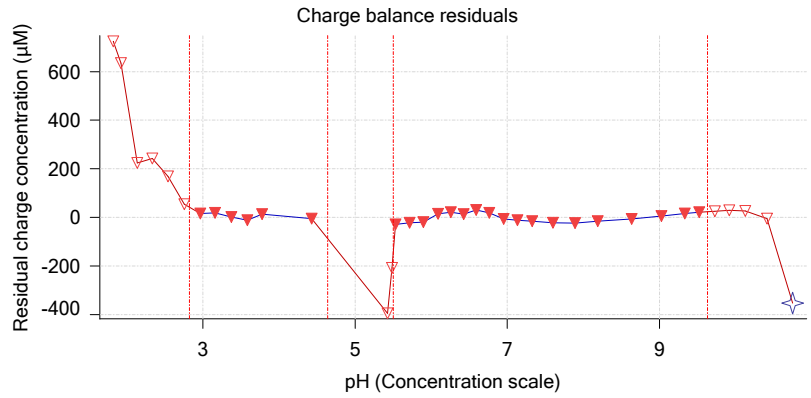


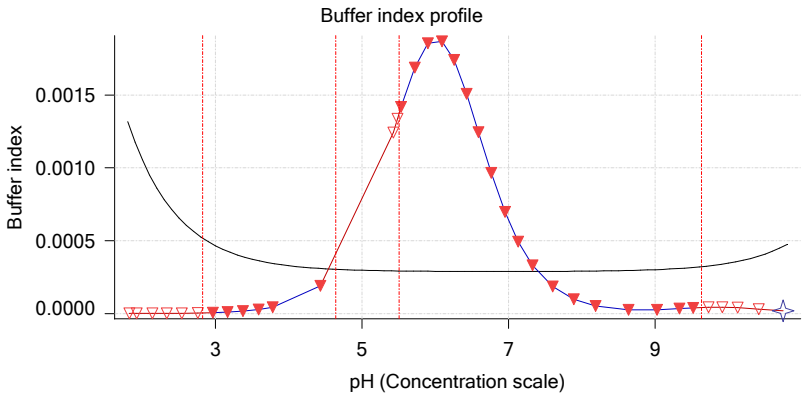


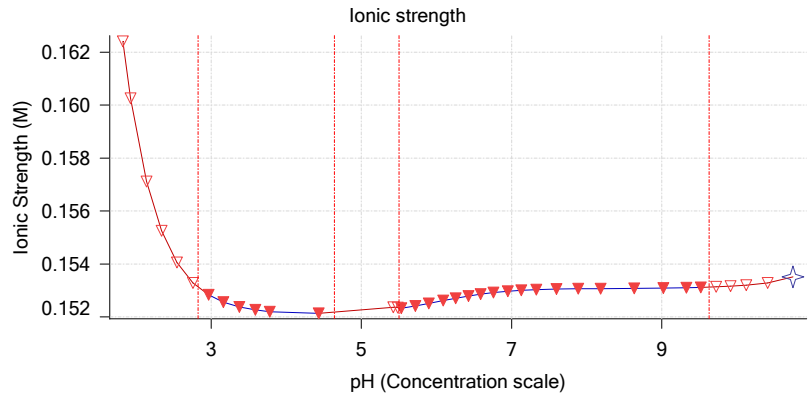
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

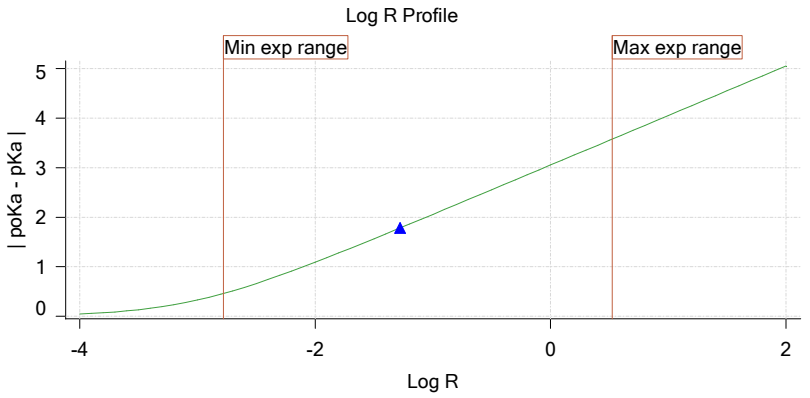
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

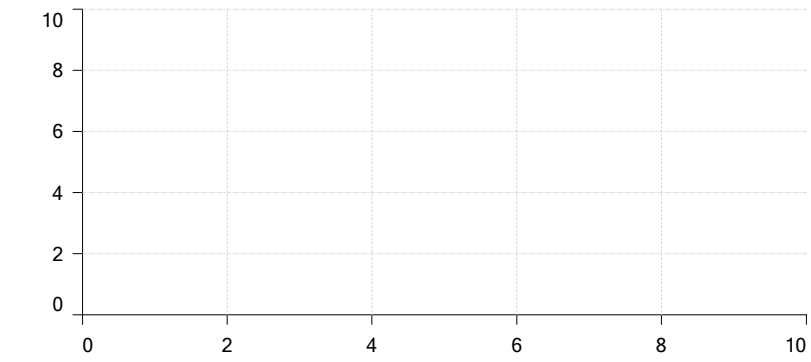
Other graphs (continued)

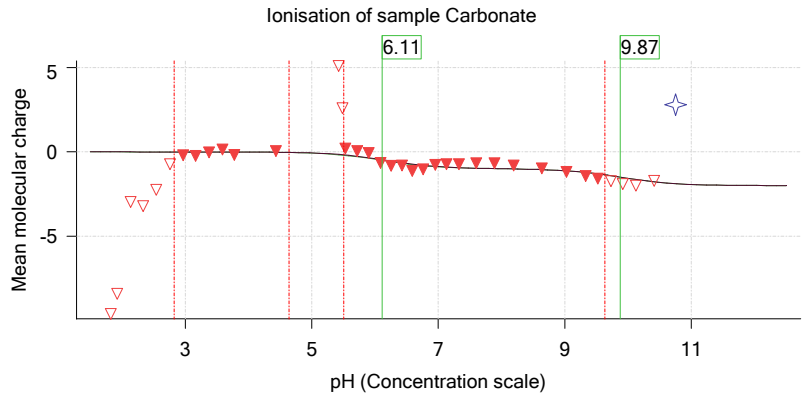












Sample name:	**M08_octanol**	Experiment start time:	**3/2/2018 5:10:52 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-02007**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18C-02007 Points 39 to 77

Overall results

RMSD	0.038
Average ionic strength	0.159 M
Average temperature	25.0°C
Partition ratio	0.1719 : 1
Analyte concentration range	2174.7 µM to 2243.9 µM
Total points considered	26 of 39

Warnings and errors

Errors	None
Warnings	One or more logP values out of range
	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r

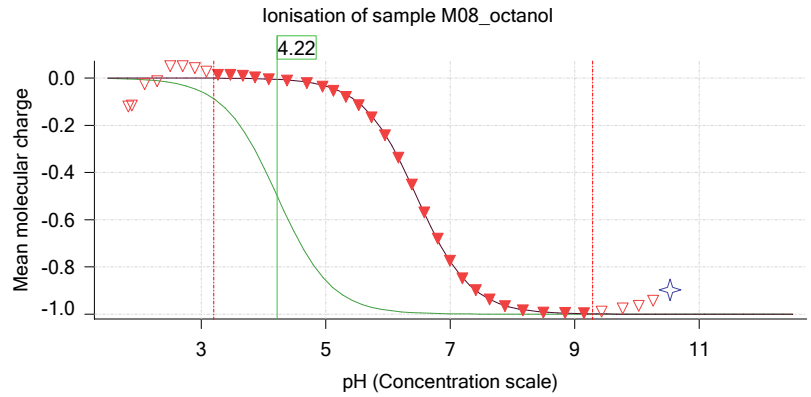
Titrants

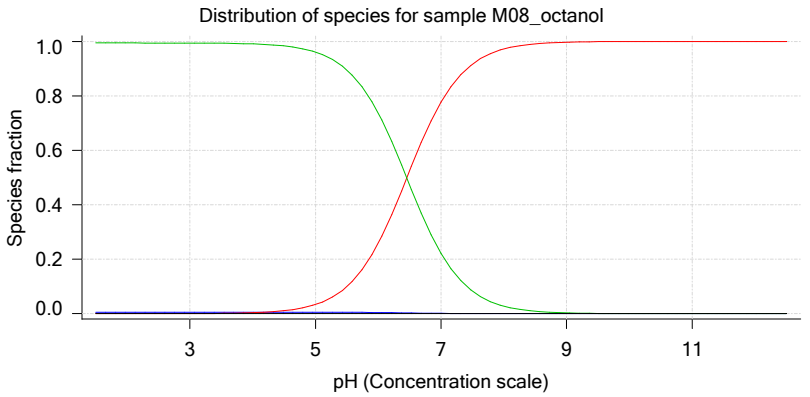
0.50 M HCl	0.999058	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 5:10:52 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor	0.855
Acid pKa 1	4.22
logP (neutral XH)	3.00
logP (X -)	-5.22

Sample graphs

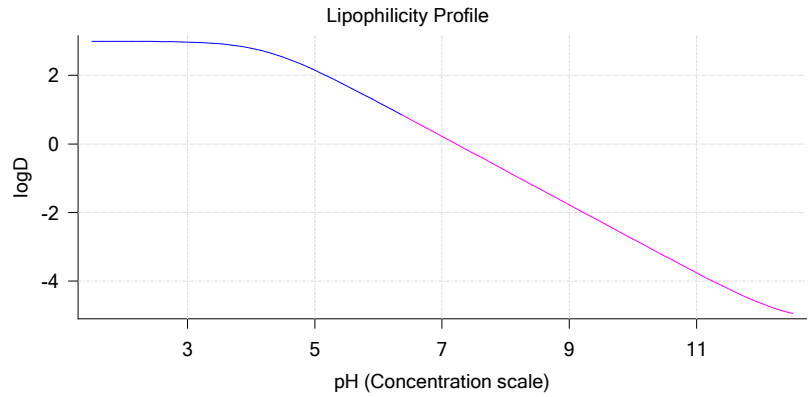




Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



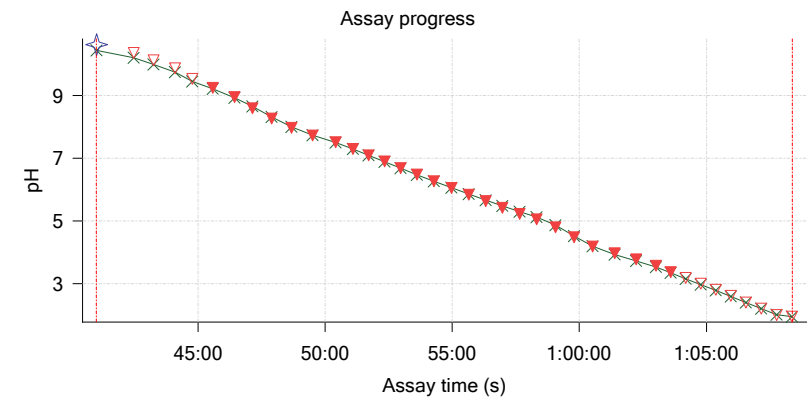
Sample logD and percent species

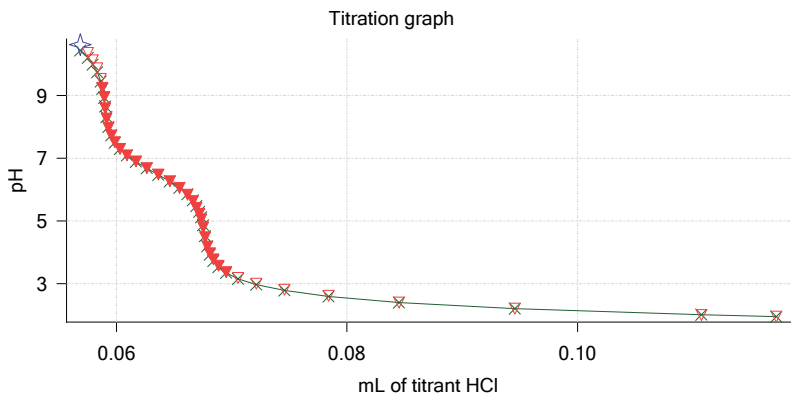
pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.00	0.58 %	0.00 %	99.42 %	0.00 %	
1.200	3.00	0.58 %	0.00 %	99.42 %	0.00 %	Stomach pH
2.000	3.00	0.58 %	0.00 %	99.42 %	0.00 %	
3.000	2.97	0.58 %	0.03 %	99.39 %	0.00 %	
4.000	2.79	0.58 %	0.35 %	99.07 %	0.00 %	
5.000	2.15	0.56 %	3.37 %	96.07 %	0.00 %	
6.000	1.21	0.43 %	25.88 %	73.69 %	0.00 %	
6.500	0.72	0.28 %	52.47 %	47.25 %	0.00 %	
7.000	0.22	0.13 %	77.74 %	22.14 %	0.00 %	
7.400	-0.18	0.06 %	89.76 %	10.18 %	0.00 %	Blood pH
8.000	-0.78	0.02 %	97.22 %	2.77 %	0.00 %	
9.000	-1.78	0.00 %	99.71 %	0.28 %	0.00 %	
10.000	-2.78	0.00 %	99.97 %	0.03 %	0.00 %	
11.000	-3.77	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.65	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.394 mM
Acidity error -1.609 mM

Other graphs

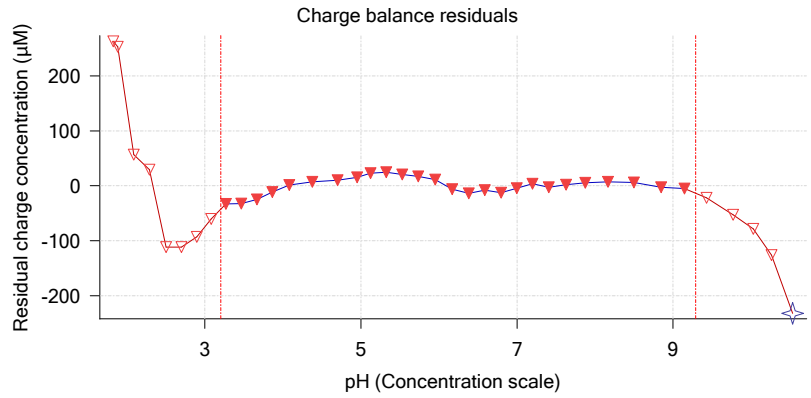


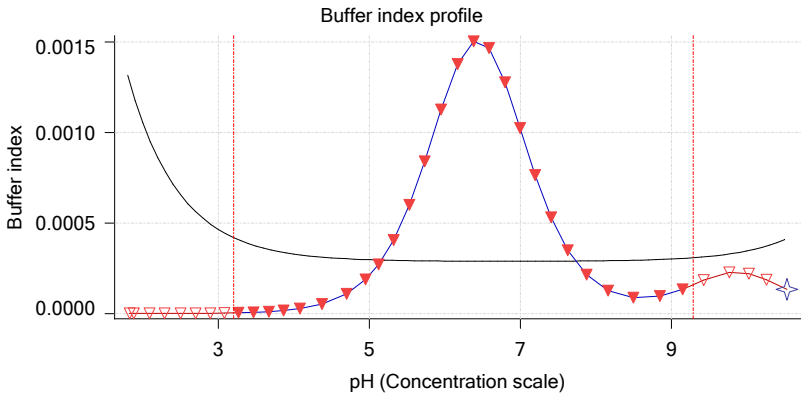


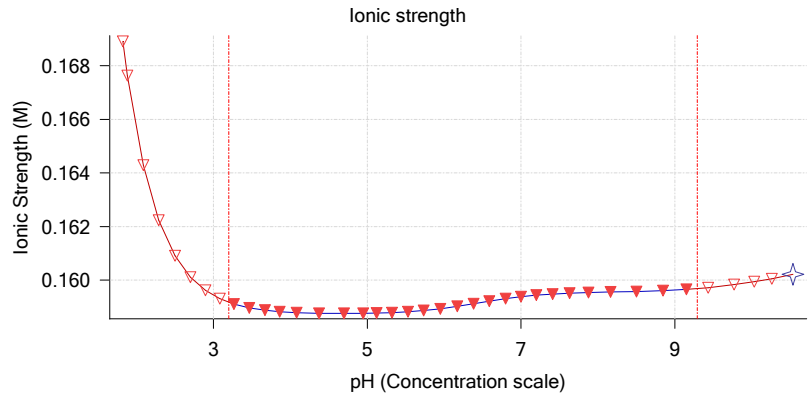
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

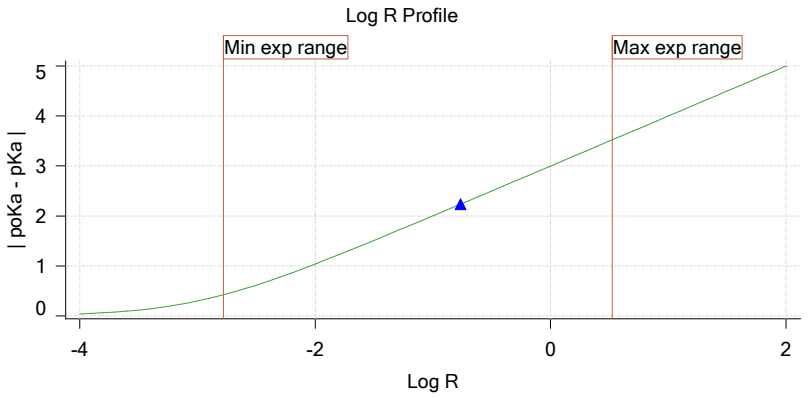
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

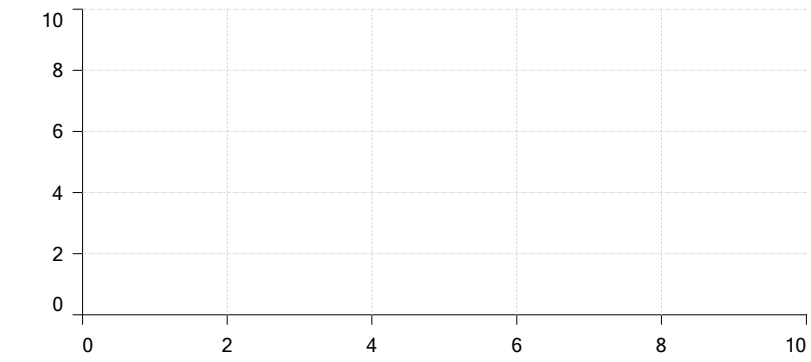
Other graphs (continued)

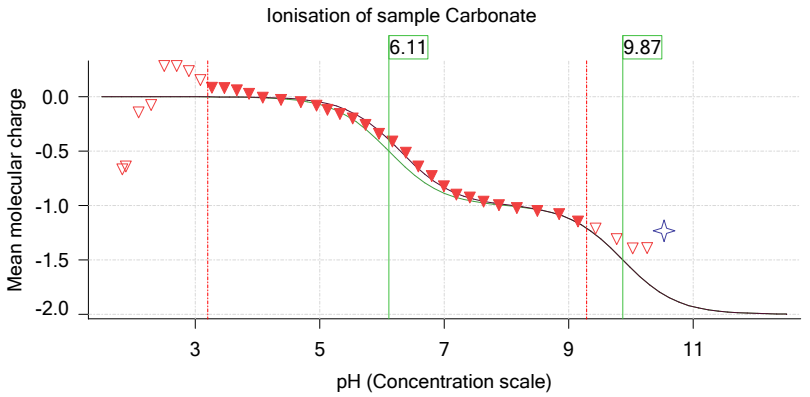












Sample name:	**M08_octanol**	Experiment start time:	**3/2/2018 5:10:52 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-02007**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18C-02007 Points 78 to 114

Overall results

RMSD	0.046
Average ionic strength	0.165 M
Average temperature	25.0°C
Partition ratio	0.6178 : 1
Analyte concentration range	1479.7 µM to 1511.5 µM
Total points considered	30 of 37

Warnings and errors

Errors	None
Warnings	One or more logP values out of range
	Excessive acidity error present

Four-Plus parameters

Alpha	0.111	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r

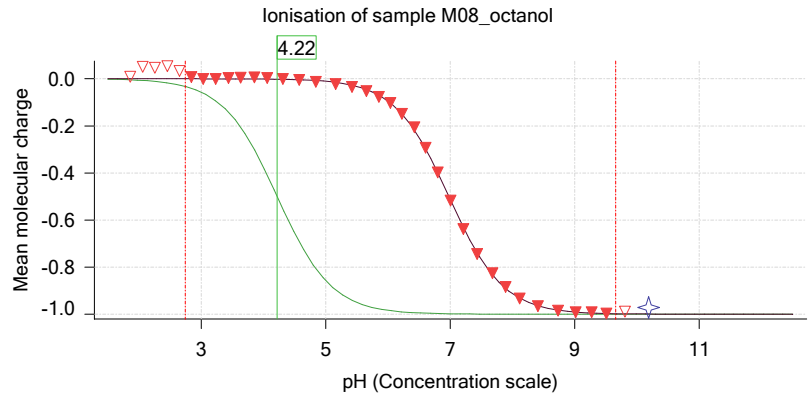
Titrants

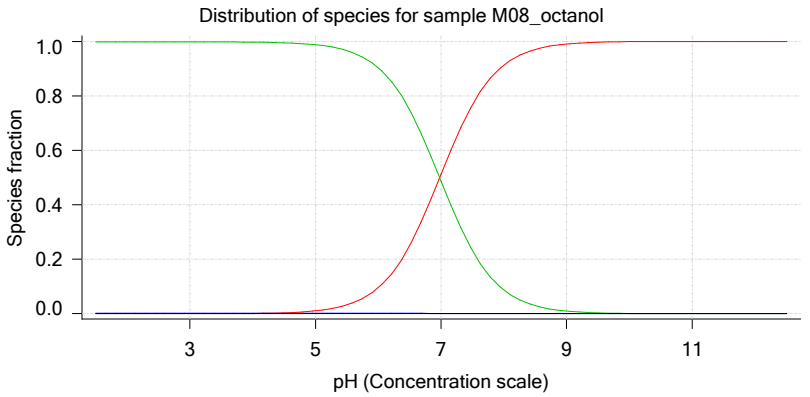
0.50 M HCl	0.999058	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 5:10:52 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor	0.850
Acid pKa 1	4.22
logP (neutral XH)	2.97
logP (X -)	-6.01

Sample graphs

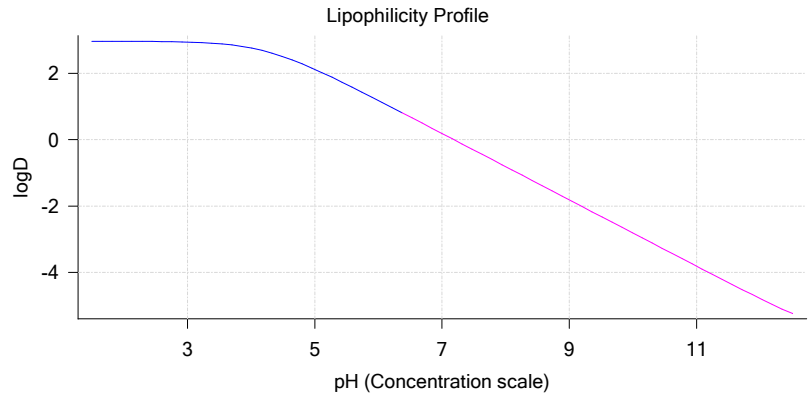




Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



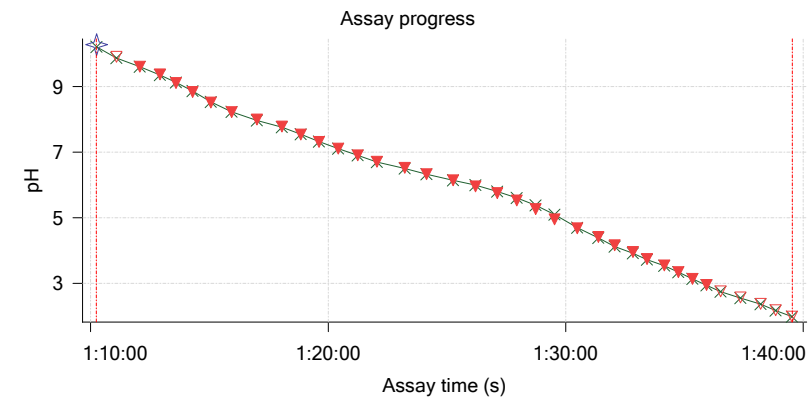
Sample logD and percent species

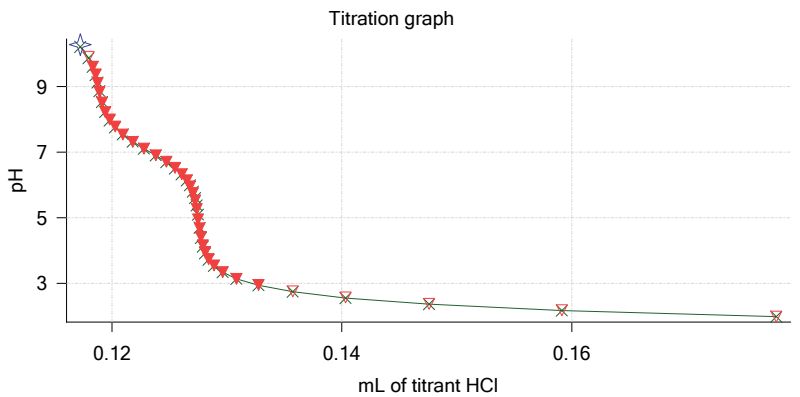
pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	2.97	0.17 %	0.00 %	99.83 %	0.00 %	
1.200	2.97	0.17 %	0.00 %	99.83 %	0.00 %	Stomach pH
2.000	2.96	0.17 %	0.00 %	99.82 %	0.00 %	
3.000	2.94	0.17 %	0.01 %	99.82 %	0.00 %	
4.000	2.76	0.17 %	0.10 %	99.72 %	0.00 %	
5.000	2.12	0.17 %	1.04 %	98.79 %	0.00 %	
6.000	1.18	0.16 %	9.50 %	90.34 %	0.00 %	
6.500	0.68	0.13 %	24.93 %	74.94 %	0.00 %	
7.000	0.19	0.09 %	51.23 %	48.69 %	0.00 %	
7.400	-0.21	0.05 %	72.51 %	27.44 %	0.00 %	Blood pH
8.000	-0.81	0.02 %	91.31 %	8.68 %	0.00 %	
9.000	-1.81	0.00 %	99.06 %	0.94 %	0.00 %	
10.000	-2.81	0.00 %	99.90 %	0.09 %	0.00 %	
11.000	-3.81	0.00 %	99.99 %	0.01 %	0.00 %	
12.000	-4.79	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.394 mM
Acidity error -1.483 mM

Other graphs

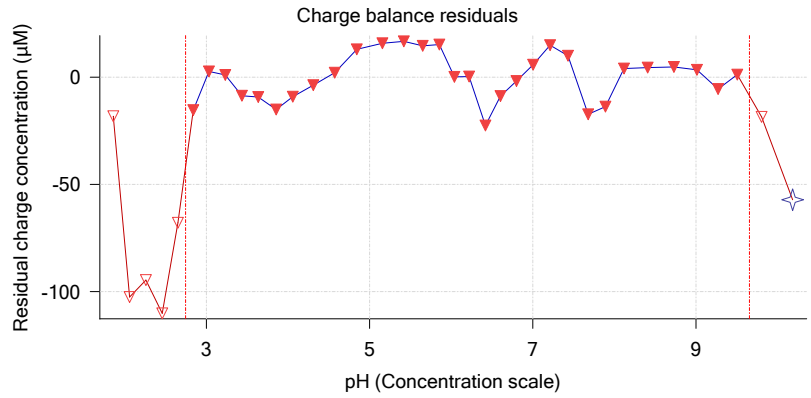


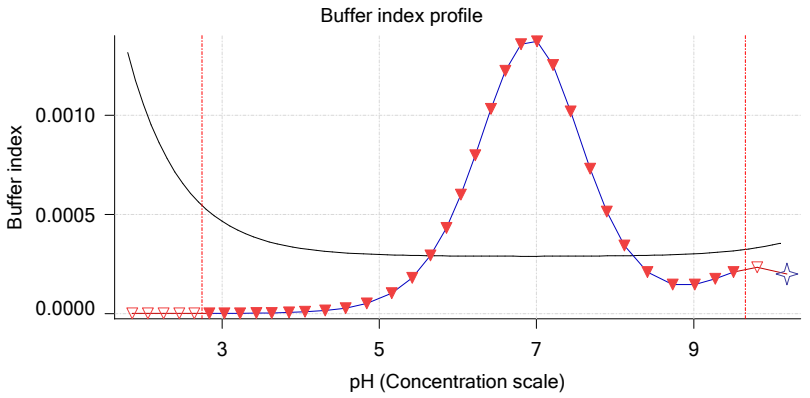


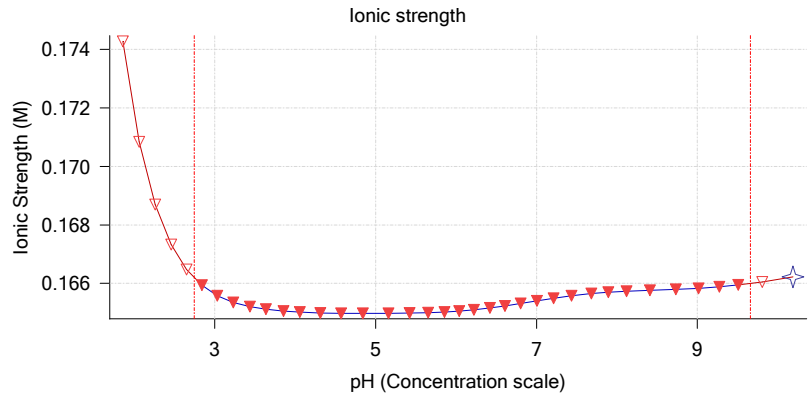
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

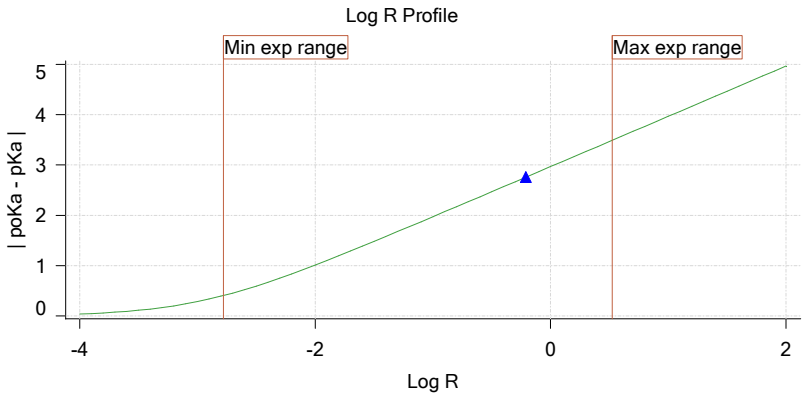
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

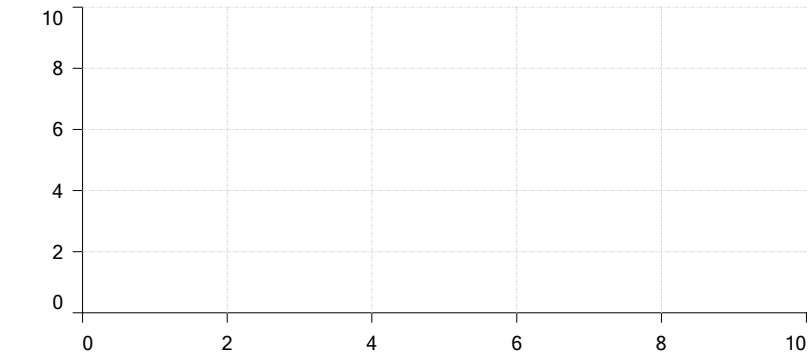
Other graphs (continued)

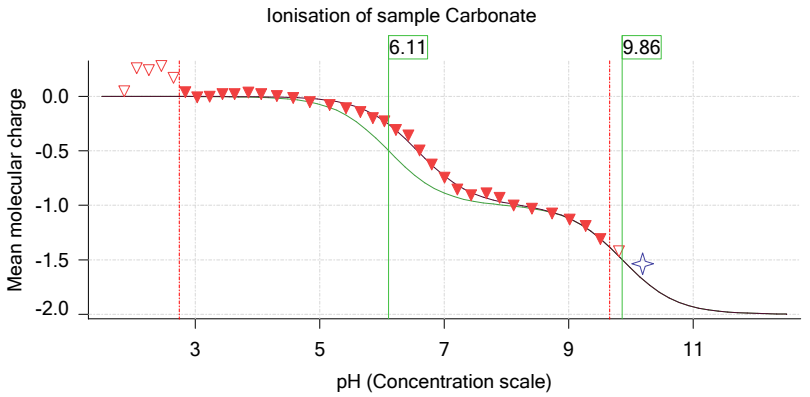












Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M08_octanol	2/27/2018 4:33:51 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001250 g	3/2/2018 5:08:08 PM	User entered value
Formula weight	293.32 g/mol	2/27/2018 4:33:51 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	293.32	2/27/2018 4:33:51 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:33:51 PM	User entered value
Sample is a	Acid	2/27/2018 4:33:51 PM	User entered value
pKa 1	4.22	2/27/2018 4:33:51 PM	User entered value
logP (neutral XH)	2.98	3/2/2018 3:22:58 PM	User entered value
logP (X -)	-5.22	3/2/2018 3:23:03 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH time
6:14.2	Manual volume addition				0.08000 mL					
6:15.3	Initial pH = 5.74									
9:07.3	Data point 2	1.50000 mL	0.00000 mL	0.00647 mL	0.08000 mL	10.845	-0.01910	0.96118	0.00097	34.5 s
10:08.5	Data point 3	1.50000 mL	0.00052 mL	0.00647 mL	0.08000 mL	10.511	0.01702	0.82617	0.00093	35.0 s
11:14.1	Data point 4	1.50000 mL	0.00108 mL	0.00647 mL	0.08000 mL	10.223	-0.01634	0.68740	0.00097	27.0 s
12:06.6	Data point 5	1.50000 mL	0.00136 mL	0.00647 mL	0.08000 mL	10.016	-0.01334	0.51589	0.00092	28.5 s
13:00.5	Data point 6	1.50000 mL	0.00155 mL	0.00647 mL	0.08000 mL	9.825	-0.01728	0.80734	0.00095	28.0 s
13:53.9	Data point 7	1.50000 mL	0.00169 mL	0.00647 mL	0.08000 mL	9.619	-0.01617	0.77696	0.00091	29.5 s
14:48.8	Data point 8	1.50000 mL	0.00179 mL	0.00647 mL	0.08000 mL	9.430	-0.01709	0.89746	0.00089	30.5 s
15:54.8	Data point 9	1.50000 mL	0.00190 mL	0.00647 mL	0.08000 mL	9.124	-0.01954	0.95895	0.00100	34.0 s
17:04.8	Data point 10	1.50000 mL	0.00200 mL	0.00647 mL	0.08000 mL	8.735	0.01424	0.54643	0.00095	10.5 s
17:50.7	Data point 11	1.50000 mL	0.00209 mL	0.00647 mL	0.08000 mL	8.289	0.01419	0.56162	0.00094	17.5 s
18:43.8	Data point 12	1.50000 mL	0.00219 mL	0.00647 mL	0.08000 mL	7.989	0.01768	0.82202	0.00096	16.0 s
19:30.3	Data point 13	1.50000 mL	0.00230 mL	0.00647 mL	0.08000 mL	7.701	0.01538	0.74821	0.00089	17.0 s
20:17.7	Data point 14	1.50000 mL	0.00249 mL	0.00647 mL	0.08000 mL	7.430	0.01705	0.74628	0.00097	16.0 s
21:09.3	Data point 15	1.50000 mL	0.00273 mL	0.00647 mL	0.08000 mL	7.233	0.01759	0.83369	0.00095	16.0 s
22:00.8	Data point 16	1.50000 mL	0.00303 mL	0.00647 mL	0.08000 mL	7.053	0.01636	0.81366	0.00091	15.5 s
22:41.9	Data point 17	1.50000 mL	0.00343 mL	0.00647 mL	0.08000 mL	6.864	0.01785	0.82800	0.00097	15.0 s
23:22.4	Data point 18	1.50000 mL	0.00397 mL	0.00647 mL	0.08000 mL	6.692	0.01764	0.77148	0.00099	14.0 s
24:12.1	Data point 19	1.50000 mL	0.00470 mL	0.00647 mL	0.08000 mL	6.530	0.01783	0.78830	0.00099	13.5 s
24:51.2	Data point 20	1.50000 mL	0.00553 mL	0.00647 mL	0.08000 mL	6.359	0.01727	0.78473	0.00097	13.0 s

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
25:29.8	Data point 21	1.50000 mL	0.00647 mL	0.00647 mL	0.08000 mL	6.192	0.01558	0.76055	0.00089	13.0 s
26:28.7	Data point 22	1.50000 mL	0.00767 mL	0.00647 mL	0.08000 mL	6.001	0.01489	0.64323	0.00092	11.0 s
27:20.5	Data point 23	1.50000 mL	0.00865 mL	0.00647 mL	0.08000 mL	5.821	0.01662	0.89411	0.00087	13.0 s
27:58.9	Data point 24	1.50000 mL	0.00955 mL	0.00647 mL	0.08000 mL	5.637	0.05313	0.99810	0.00262	Timed out at 59.0 s
29:24.2	Data point 25	1.50000 mL	0.01030 mL	0.00647 mL	0.08000 mL	5.588	0.13136	0.99843	0.00649	Timed out at 59.5 s
31:00.0	Data point 26	1.50000 mL	0.01110 mL	0.00647 mL	0.08000 mL	5.531	0.09941	0.99750	0.00492	Timed out at 59.5 s
32:25.5	Data point 27	1.50000 mL	0.01183 mL	0.00647 mL	0.08000 mL	4.537	0.01986	0.98034	0.00099	49.0 s
33:45.2	Data point 28	1.50000 mL	0.01237 mL	0.00647 mL	0.08000 mL	3.885	0.01681	0.92569	0.00086	11.5 s
34:32.4	Data point 29	1.50000 mL	0.01275 mL	0.00647 mL	0.08000 mL	3.693	0.00140	0.02989	0.00040	10.0 s
35:08.0	Data point 30	1.50000 mL	0.01322 mL	0.00647 mL	0.08000 mL	3.482	0.01095	0.91600	0.00057	10.0 s
35:43.5	Data point 31	1.50000 mL	0.01399 mL	0.00647 mL	0.08000 mL	3.270	0.00378	0.79588	0.00021	10.0 s
36:19.0	Data point 32	1.50000 mL	0.01522 mL	0.00647 mL	0.08000 mL	3.073	-0.00000	0.00000	0.00009	10.0 s
36:54.5	Data point 33	1.50000 mL	0.01714 mL	0.00647 mL	0.08000 mL	2.866	-0.00657	0.26783	0.00063	10.0 s
37:30.0	Data point 34	1.50000 mL	0.02027 mL	0.00647 mL	0.08000 mL	2.651	-0.00505	0.84244	0.00027	10.0 s
38:05.6	Data point 35	1.50000 mL	0.02542 mL	0.00647 mL	0.08000 mL	2.448	-0.00911	0.70428	0.00054	10.0 s
38:41.2	Data point 36	1.50000 mL	0.03380 mL	0.00647 mL	0.08000 mL	2.253	-0.00829	0.95487	0.00042	10.5 s
39:17.3	Data point 37	1.50000 mL	0.04713 mL	0.00647 mL	0.08000 mL	2.045	-0.00957	0.94345	0.00049	10.5 s
39:53.4	Data point 38	1.50000 mL	0.05687 mL	0.00647 mL	0.08000 mL	1.947	-0.01349	0.79563	0.00075	10.0 s
41:01.1	Data point 39	1.50000 mL	0.05687 mL	0.06235 mL	0.28000 mL	10.631	-0.01759	0.84525	0.00094	46.5 s
42:28.5	Data point 40	1.50000 mL	0.05753 mL	0.06235 mL	0.28000 mL	10.359	-0.01582	0.80255	0.00087	21.0 s
43:14.9	Data point 41	1.50000 mL	0.05795 mL	0.06235 mL	0.28000 mL	10.128	-0.01731	0.77064	0.00098	20.5 s
44:06.0	Data point 42	1.50000 mL	0.05833 mL	0.06235 mL	0.28000 mL	9.868	-0.01482	0.86960	0.00079	10.0 s
44:46.6	Data point 43	1.50000 mL	0.05863 mL	0.06235 mL	0.28000 mL	9.530	0.01648	0.70393	0.00097	18.0 s
45:35.3	Data point 44	1.50000 mL	0.05880 mL	0.06235 mL	0.28000 mL	9.248	0.00953	0.92650	0.00049	10.0 s
46:26.1	Data point 45	1.50000 mL	0.05894 mL	0.06235 mL	0.28000 mL	8.947	0.01716	0.79689	0.00095	12.0 s
47:08.7	Data point 46	1.50000 mL	0.05903 mL	0.06235 mL	0.28000 mL	8.599	0.01796	0.79610	0.00099	15.0 s
47:54.2	Data point 47	1.50000 mL	0.05915 mL	0.06235 mL	0.28000 mL	8.266	0.01550	0.73917	0.00089	16.0 s
48:40.8	Data point 48	1.50000 mL	0.05931 mL	0.06235 mL	0.28000 mL	7.978	0.01748	0.85525	0.00093	14.5 s
49:30.9	Data point 49	1.50000 mL	0.05955 mL	0.06235 mL	0.28000 mL	7.732	0.01742	0.81873	0.00095	13.5 s
50:25.3	Data point 50	1.50000 mL	0.05988 mL	0.06235 mL	0.28000 mL	7.511	0.01772	0.84280	0.00095	15.0 s
51:05.7	Data point 51	1.50000 mL	0.06030 mL	0.06235 mL	0.28000 mL	7.300	0.01794	0.80992	0.00098	12.0 s
51:43.1	Data point 52	1.50000 mL	0.06091 mL	0.06235 mL	0.28000 mL	7.099	0.01591	0.80910	0.00087	12.0 s
52:20.5	Data point 53	1.50000 mL	0.06169 mL	0.06235 mL	0.28000 mL	6.900	0.01723	0.80221	0.00095	12.5 s
52:58.5	Data point 54	1.50000 mL	0.06263 mL	0.06235 mL	0.28000 mL	6.688	0.01881	0.86957	0.00100	12.5 s
53:36.4	Data point 55	1.50000 mL	0.06364 mL	0.06235 mL	0.28000 mL	6.485	0.01949	0.96513	0.00098	14.5 s
54:16.5	Data point 56	1.50000 mL	0.06463 mL	0.06235 mL	0.28000 mL	6.272	0.01746	0.81817	0.00095	16.0 s
54:58.0	Data point 57	1.50000 mL	0.06548 mL	0.06235 mL	0.28000 mL	6.054	0.01509	0.72773	0.00087	15.5 s
55:38.9	Data point 58	1.50000 mL	0.06616 mL	0.06235 mL	0.28000 mL	5.836	0.01598	0.67878	0.00096	14.5 s
56:18.8	Data point 59	1.50000 mL	0.06663 mL	0.06235 mL	0.28000 mL	5.633	0.01711	0.75074	0.00098	14.5 s
56:58.7	Data point 60	1.50000 mL	0.06696 mL	0.06235 mL	0.28000 mL	5.426	0.01163	0.43580	0.00087	15.0 s
57:39.1	Data point 61	1.50000 mL	0.06719 mL	0.06235 mL	0.28000 mL	5.227	0.01748	0.74548	0.00100	14.5 s
58:19.1	Data point 62	1.50000 mL	0.06736 mL	0.06235 mL	0.28000 mL	5.053	0.01418	0.59508	0.00091	14.0 s
59:03.7	Data point 63	1.50000 mL	0.06752 mL	0.06235 mL	0.28000 mL	4.804	0.01416	0.51436	0.00098	13.0 s
59:47.2	Data point 64	1.50000 mL	0.06769 mL	0.06235 mL	0.28000 mL	4.481	-0.01418	0.54917	0.00095	13.5 s
1:00:31.3	Data point 65	1.50000 mL	0.06787 mL	0.06235 mL	0.28000 mL	4.188	0.00796	0.27623	0.00075	11.5 s
1:01:23.6	Data point 66	1.50000 mL	0.06811 mL	0.06235 mL	0.28000 mL	3.970	0.00985	0.32707	0.00085	10.0 s
1:02:14.3	Data point 67	1.50000 mL	0.06841 mL	0.06235 mL	0.28000 mL	3.775	0.00616	0.11203	0.00091	10.5 s
1:03:00.6	Data point 68	1.50000 mL	0.06886 mL	0.06235 mL	0.28000 mL	3.573	-0.00222	0.09420	0.00036	10.0 s
1:03:36.0	Data point 69	1.50000 mL	0.06952 mL	0.06235 mL	0.28000 mL	3.375	-0.00763	0.55206	0.00051	10.0 s
1:04:11.4	Data point 70	1.50000 mL	0.07056 mL	0.06235 mL	0.28000 mL	3.190	-0.00162	0.01741	0.00061	10.0 s
1:04:46.9	Data point 71	1.50000 mL	0.07213 mL	0.06235 mL	0.28000 mL	3.003	-0.00478	0.16896	0.00058	10.0 s
1:05:22.5	Data point 72	1.50000 mL	0.07458 mL	0.06235 mL	0.28000 mL	2.809	-0.01075	0.85851	0.00057	10.0 s
1:05:57.9	Data point 73	1.50000 mL	0.07841 mL	0.06235 mL	0.28000 mL	2.612	-0.00808	0.55458	0.00054	10.0 s
1:06:33.4	Data point 74	1.50000 mL	0.08452 mL	0.06235 mL	0.28000 mL	2.403	-0.01513	0.90224	0.00079	10.5 s

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:07:09.6	Data point 75	1.50000 mL	0.09457 mL	0.06235 mL	0.28000 mL	2.205	-0.01575	0.80047	0.00087	10.5 s
1:07:46.0	Data point 76	1.50000 mL	0.11075 mL	0.06235 mL	0.28000 mL	2.005	-0.01140	0.94279	0.00058	10.0 s
1:08:21.6	Data point 77	1.50000 mL	0.11724 mL	0.06235 mL	0.28000 mL	1.949	-0.01059	0.59925	0.00068	10.5 s
1:10:15.2	Data point 78	1.50000 mL	0.11724 mL	0.12227 mL	1.08000 mL	10.284	-0.01559	0.68044	0.00093	19.0 s
1:11:04.8	Data point 79	1.50000 mL	0.11797 mL	0.12227 mL	1.08000 mL	9.905	-0.01823	0.85938	0.00097	29.0 s
1:12:04.4	Data point 80	1.50000 mL	0.11832 mL	0.12227 mL	1.08000 mL	9.606	0.00322	0.20225	0.00035	10.0 s
1:12:55.2	Data point 81	1.50000 mL	0.11858 mL	0.12227 mL	1.08000 mL	9.372	0.01018	0.33175	0.00087	10.0 s
1:13:35.8	Data point 82	1.50000 mL	0.11874 mL	0.12227 mL	1.08000 mL	9.113	0.01675	0.72883	0.00097	11.5 s
1:14:17.8	Data point 83	1.50000 mL	0.11891 mL	0.12227 mL	1.08000 mL	8.833	0.01720	0.72480	0.00100	15.0 s
1:15:03.3	Data point 84	1.50000 mL	0.11912 mL	0.12227 mL	1.08000 mL	8.510	0.01867	0.92540	0.00096	22.0 s
1:15:55.9	Data point 85	1.50000 mL	0.11940 mL	0.12227 mL	1.08000 mL	8.218	0.01492	0.63364	0.00092	23.5 s
1:17:00.2	Data point 86	1.50000 mL	0.11980 mL	0.12227 mL	1.08000 mL	7.993	0.01343	0.47459	0.00096	22.0 s
1:18:03.1	Data point 87	1.50000 mL	0.12027 mL	0.12227 mL	1.08000 mL	7.782	0.00779	0.17186	0.00093	22.5 s
1:18:51.0	Data point 88	1.50000 mL	0.12093 mL	0.12227 mL	1.08000 mL	7.536	0.01513	0.63465	0.00094	20.5 s
1:19:36.9	Data point 89	1.50000 mL	0.12180 mL	0.12227 mL	1.08000 mL	7.314	0.01545	0.64305	0.00095	23.0 s
1:20:25.4	Data point 90	1.50000 mL	0.12279 mL	0.12227 mL	1.08000 mL	7.108	0.01486	0.61616	0.00093	24.0 s
1:21:14.9	Data point 91	1.50000 mL	0.12380 mL	0.12227 mL	1.08000 mL	6.904	0.01585	0.65380	0.00097	23.0 s
1:22:03.3	Data point 92	1.50000 mL	0.12472 mL	0.12227 mL	1.08000 mL	6.708	0.01765	0.76772	0.00100	29.0 s
1:23:13.3	Data point 93	1.50000 mL	0.12549 mL	0.12227 mL	1.08000 mL	6.525	0.01641	0.69561	0.00097	29.5 s
1:24:08.2	Data point 94	1.50000 mL	0.12606 mL	0.12227 mL	1.08000 mL	6.325	0.01752	0.80208	0.00097	31.5 s
1:25:15.4	Data point 95	1.50000 mL	0.12651 mL	0.12227 mL	1.08000 mL	6.143	0.01142	0.37473	0.00092	31.5 s
1:26:12.4	Data point 96	1.50000 mL	0.12679 mL	0.12227 mL	1.08000 mL	5.958	0.01161	0.45352	0.00085	19.0 s
1:27:07.1	Data point 97	1.50000 mL	0.12705 mL	0.12227 mL	1.08000 mL	5.756	0.01128	0.44370	0.00084	18.5 s
1:27:56.1	Data point 98	1.50000 mL	0.12723 mL	0.12227 mL	1.08000 mL	5.523	0.00514	0.07395	0.00093	17.5 s
1:28:44.2	Data point 99	1.50000 mL	0.12737 mL	0.12227 mL	1.08000 mL	5.263	0.00888	0.39531	0.00070	17.0 s
1:29:31.7	Data point 100	1.50000 mL	0.12749 mL	0.12227 mL	1.08000 mL	4.946	0.01013	0.28860	0.00093	22.0 s
1:30:29.4	Data point 101	1.50000 mL	0.12761 mL	0.12227 mL	1.08000 mL	4.676	0.01394	0.55015	0.00093	17.5 s
1:31:22.6	Data point 102	1.50000 mL	0.12773 mL	0.12227 mL	1.08000 mL	4.416	0.01242	0.40861	0.00096	11.0 s
1:32:04.1	Data point 103	1.50000 mL	0.12789 mL	0.12227 mL	1.08000 mL	4.164	0.00814	0.19383	0.00091	10.0 s
1:32:49.9	Data point 104	1.50000 mL	0.12810 mL	0.12227 mL	1.08000 mL	3.959	0.00234	0.03684	0.00060	10.0 s
1:33:25.3	Data point 105	1.50000 mL	0.12841 mL	0.12227 mL	1.08000 mL	3.741	-0.01363	0.76827	0.00077	18.5 s
1:34:09.1	Data point 106	1.50000 mL	0.12888 mL	0.12227 mL	1.08000 mL	3.543	-0.01018	0.83349	0.00055	10.0 s
1:34:44.5	Data point 107	1.50000 mL	0.12963 mL	0.12227 mL	1.08000 mL	3.337	-0.01423	0.90918	0.00074	10.0 s
1:35:20.0	Data point 108	1.50000 mL	0.13083 mL	0.12227 mL	1.08000 mL	3.139	-0.01823	0.90719	0.00095	10.0 s
1:35:55.6	Data point 109	1.50000 mL	0.13274 mL	0.12227 mL	1.08000 mL	2.947	-0.01750	0.91940	0.00090	10.0 s
1:36:31.1	Data point 110	1.50000 mL	0.13572 mL	0.12227 mL	1.08000 mL	2.759	-0.01737	0.77482	0.00097	24.5 s
1:37:21.2	Data point 111	1.50000 mL	0.14033 mL	0.12227 mL	1.08000 mL	2.568	-0.01758	0.81168	0.00096	25.5 s
1:38:12.4	Data point 112	1.50000 mL	0.14758 mL	0.12227 mL	1.08000 mL	2.370	-0.01653	0.73042	0.00096	12.0 s
1:38:50.1	Data point 113	1.50000 mL	0.15915 mL	0.12227 mL	1.08000 mL	2.176	-0.01588	0.71562	0.00093	15.5 s
1:39:31.5	Data point 114	1.50000 mL	0.17780 mL	0.12227 mL	1.08000 mL	1.980	-0.01565	0.88128	0.00082	11.5 s
1:39:52.1	Assay volumes	1.50000 mL	0.17780 mL	0.12227 mL	1.08000 mL					

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.080 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	High to low pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.800 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/2/2018 5:10:52 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/2/2018 5:10:52 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.92 mV		3/2/2018 5:11:36 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	7.4e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.1e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**
Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[1:59] Air gap released for Acid (0.5 M HCl)
[2:54] Air gap created for Water (0.15 M KCl)
[2:54] Air gap created for Acid (0.5 M HCl)
[2:55] Air gap created for Base (0.5 M KOH)
[2:55] Air gap released for Water (0.15 M KCl)
[2:59] Titrator arm moved over Titration position
[2:59] Titration 1 of 3
[2:59] Adding initial titrants
[2:59] Automatically add 1.50000 mL of water
[3:24] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:28] Titrator arm moved over Drain
[6:09] Titrator arm moved to Titration position
[6:09] Argon flow rate set to 100
[6:09] Stirrer speed set to 10
[6:16] Initial pH = 5.74
[6:16] Iterative adjust 5.74 -> 10.00
[6:16] pH 5.74 -> 10.00
[6:16] Air gap released for Base (0.5 M KOH)
[6:17] Dispensed 0.006468 mL of Base (0.5 M KOH)
[6:22] Holding pH 10.00
[8:22] Stirrer speed set to 0
[8:22] Stirrer speed set to 50
[8:22] Iterative adjust 11.25 -> 10.00
[9:07] Stirrer speed set to 0
[9:42] Datapoint id 2 collected
[9:42] Stirrer speed set to 50
[9:47] pH 10.83 -> 10.63
[9:47] Using cautious pH adjust
[9:48] Air gap released for Acid (0.5 M HCl)
[9:49] Dispensed 0.000517 mL of Acid (0.5 M HCl)
[9:54] Stepping pH = 10.62
[10:09] Stirrer speed set to 0
[10:44] Datapoint id 3 collected
[10:44] Charge balance equation is out by 50.1%
[10:44] Stirrer speed set to 50
[10:49] pH 10.50 -> 10.30
[10:49] Using cautious pH adjust
[10:49] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[10:54] Stepping pH = 10.44
[10:54] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[10:59] Stepping pH = 10.31
[11:14] Stirrer speed set to 0

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[11:41] Datapoint id 4 collected
[11:41] Charge balance equation is out by -9.4%
[11:41] Stirrer speed set to 50
[11:46] pH 10.22 -> 10.02
[11:46] Using charge balance adjust
[11:47] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[12:07] Stirrer speed set to 0
[12:35] Datapoint id 5 collected
[12:35] Charge balance equation is out by 4.0%
[12:35] Stirrer speed set to 50
[12:40] pH 10.00 -> 9.80
[12:40] Using charge balance adjust
[12:40] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[13:01] Stirrer speed set to 0
[13:29] Datapoint id 6 collected
[13:29] Charge balance equation is out by -10.5%
[13:29] Stirrer speed set to 50
[13:34] pH 9.81 -> 9.61
[13:34] Using charge balance adjust
[13:34] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[13:54] Stirrer speed set to 0
[14:24] Datapoint id 7 collected
[14:24] Charge balance equation is out by -4.1%
[14:24] Stirrer speed set to 50
[14:29] pH 9.60 -> 9.40
[14:29] Using charge balance adjust
[14:29] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[14:49] Stirrer speed set to 0
[15:20] Datapoint id 8 collected
[15:20] Charge balance equation is out by -16.0%
[15:20] Stirrer speed set to 50
[15:25] pH 9.40 -> 9.20
[15:25] Using cautious pH adjust
[15:25] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[15:30] Stepping pH = 9.38
[15:30] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[15:35] Stepping pH = 9.22
[15:35] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[15:40] Stepping pH = 9.17
[15:55] Stirrer speed set to 0
[16:29] Datapoint id 9 collected
[16:29] Charge balance equation is out by -121.4%
[16:29] Stirrer speed set to 50
[16:34] pH 9.07 -> 8.87
[16:34] Using cautious pH adjust
[16:34] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[16:40] Stepping pH = 9.05
[16:40] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[16:45] Stepping pH = 8.91
[16:45] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[16:50] Stepping pH = 8.80
[17:05] Stirrer speed set to 0
[17:15] Datapoint id 10 collected
[17:15] Charge balance equation is out by -150.8%
[17:15] Stirrer speed set to 50
[17:20] pH 8.72 -> 8.52
[17:20] Using cautious pH adjust
[17:21] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[17:26] Stepping pH = 8.71

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:26] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[17:31] Stepping pH = 8.66
[17:31] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[17:36] Stepping pH = 8.37
[17:51] Stirrer speed set to 0
[18:08] Datapoint id 11 collected
[18:08] Charge balance equation is out by -335.3%
[18:08] Stirrer speed set to 50
[18:13] pH 8.27 -> 8.07
[18:13] Using cautious pH adjust
[18:14] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[18:19] Stepping pH = 8.26
[18:19] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[18:24] Stepping pH = 8.12
[18:24] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[18:29] Stepping pH = 8.04
[18:44] Stirrer speed set to 0
[19:00] Datapoint id 12 collected
[19:00] Charge balance equation is out by -155.8%
[19:00] Stirrer speed set to 50
[19:05] pH 7.96 -> 7.76
[19:05] Using cautious pH adjust
[19:05] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[19:10] Stepping pH = 7.95
[19:10] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[19:15] Stepping pH = 7.75
[19:31] Stirrer speed set to 0
[19:48] Datapoint id 13 collected
[19:48] Charge balance equation is out by -93.4%
[19:48] Stirrer speed set to 50
[19:53] pH 7.69 -> 7.49
[19:53] Using cautious pH adjust
[19:53] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[19:58] Stepping pH = 7.66
[19:58] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[20:03] Stepping pH = 7.44
[20:18] Stirrer speed set to 0
[20:34] Datapoint id 14 collected
[20:34] Charge balance equation is out by -74.1%
[20:34] Stirrer speed set to 50
[20:39] pH 7.42 -> 7.22
[20:39] Using cautious pH adjust
[20:39] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[20:44] Stepping pH = 7.35
[20:44] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[20:49] Stepping pH = 7.23
[20:49] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[20:54] Stepping pH = 7.22
[21:10] Stirrer speed set to 0
[21:26] Datapoint id 15 collected
[21:26] Charge balance equation is out by -18.8%
[21:26] Stirrer speed set to 50
[21:31] pH 7.22 -> 7.02
[21:31] Using cautious pH adjust
[21:31] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[21:36] Stepping pH = 7.12
[21:36] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[21:41] Stepping pH = 7.07
[21:41] Dispensed 0.000071 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:46] Stepping pH = 7.03
[22:01] Stirrer speed set to 0
[22:17] Datapoint id 16 collected
[22:17] Charge balance equation is out by -9.3%
[22:17] Stirrer speed set to 50
[22:22] pH 7.05 -> 6.85
[22:22] Using charge balance adjust
[22:22] Dispensed 0.000400 mL of Acid (0.5 M HCl)
[22:42] Stirrer speed set to 0
[22:57] Datapoint id 17 collected
[22:57] Charge balance equation is out by -6.8%
[22:57] Stirrer speed set to 50
[23:02] pH 6.86 -> 6.66
[23:02] Using charge balance adjust
[23:02] Dispensed 0.000541 mL of Acid (0.5 M HCl)
[23:23] Stirrer speed set to 0
[23:37] Datapoint id 18 collected
[23:37] Charge balance equation is out by -17.6%
[23:37] Stirrer speed set to 50
[23:42] pH 6.69 -> 6.49
[23:42] Using cautious pH adjust
[23:42] Dispensed 0.000353 mL of Acid (0.5 M HCl)
[23:47] Stepping pH = 6.57
[23:47] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[23:52] Stepping pH = 6.54
[23:52] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[23:57] Stepping pH = 6.50
[24:12] Stirrer speed set to 0
[24:26] Datapoint id 19 collected
[24:26] Charge balance equation is out by -4.7%
[24:26] Stirrer speed set to 50
[24:31] pH 6.53 -> 6.33
[24:31] Using charge balance adjust
[24:31] Dispensed 0.000823 mL of Acid (0.5 M HCl)
[24:51] Stirrer speed set to 0
[25:05] Datapoint id 20 collected
[25:05] Charge balance equation is out by -13.9%
[25:05] Stirrer speed set to 50
[25:10] pH 6.36 -> 6.16
[25:10] Using charge balance adjust
[25:10] Dispensed 0.000941 mL of Acid (0.5 M HCl)
[25:30] Stirrer speed set to 0
[25:43] Datapoint id 21 collected
[25:43] Charge balance equation is out by -17.0%
[25:43] Stirrer speed set to 50
[25:48] pH 6.19 -> 5.99
[25:48] Using cautious pH adjust
[25:48] Dispensed 0.000494 mL of Acid (0.5 M HCl)
[25:53] Stepping pH = 6.09
[25:53] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[25:59] Stepping pH = 6.04
[25:59] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[26:04] Stepping pH = 6.01
[26:04] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[26:09] Stepping pH = 6.00
[26:09] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[26:14] Stepping pH = 5.99
[26:29] Stirrer speed set to 0
[26:40] Datapoint id 22 collected

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[26:40] Charge balance equation is out by -22.6%
[26:40] Stirrer speed set to 50
[26:45] pH 6.00 -> 5.80
[26:45] Using cautious pH adjust
[26:45] Dispensed 0.000494 mL of Acid (0.5 M HCl)
[26:50] Stepping pH = 5.88
[26:50] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[26:55] Stepping pH = 5.85
[26:55] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[27:00] Stepping pH = 5.82
[27:01] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[27:06] Stepping pH = 5.81
[27:21] Stirrer speed set to 0
[27:34] Datapoint id 23 collected
[27:34] Charge balance equation is out by -0.9%
[27:34] Stirrer speed set to 50
[27:39] pH 5.82 -> 5.62
[27:39] Using charge balance adjust
[27:39] Dispensed 0.000894 mL of Acid (0.5 M HCl)
[27:59] Stirrer speed set to 0
[28:59] Datapoint id 24 collected
[28:59] Charge balance equation is out by -7.3%
[28:59] Stirrer speed set to 50
[29:04] pH 5.65 -> 5.45
[29:04] Using charge balance adjust
[29:04] Dispensed 0.000753 mL of Acid (0.5 M HCl)
[29:24] Stirrer speed set to 0
[30:24] Datapoint id 25 collected
[30:24] Charge balance equation is out by -68.1%
[30:24] Stirrer speed set to 50
[30:30] pH 5.66 -> 5.46
[30:30] Using cautious pH adjust
[30:30] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[30:35] Stepping pH = 5.52
[30:35] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[30:40] Stepping pH = 5.51
[30:40] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[30:45] Stepping pH = 5.31
[31:00] Stirrer speed set to 0
[32:00] Datapoint id 26 collected
[32:00] Charge balance equation is out by -6.1%
[32:00] Stirrer speed set to 50
[32:05] pH 5.62 -> 5.42
[32:05] Using charge balance adjust
[32:06] Dispensed 0.000729 mL of Acid (0.5 M HCl)
[32:26] Stirrer speed set to 0
[33:15] Datapoint id 27 collected
[33:15] Charge balance equation is out by 443.4%
[33:15] Stirrer speed set to 50
[33:20] pH 4.60 -> 4.40
[33:20] Using cautious pH adjust
[33:20] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[33:25] Stepping pH = 4.61
[33:25] Dispensed 0.000447 mL of Acid (0.5 M HCl)
[33:30] Stepping pH = 3.88
[33:45] Stirrer speed set to 0
[33:57] Datapoint id 28 collected
[33:57] Charge balance equation is out by -208.0%
[33:57] Stirrer speed set to 50

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[34:02] pH 3.89 -> 3.69
[34:02] Using cautious pH adjust
[34:02] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[34:07] Stepping pH = 3.81
[34:07] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[34:12] Stepping pH = 3.70
[34:12] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[34:18] Stepping pH = 3.70
[34:33] Stirrer speed set to 0
[34:43] Datapoint id 29 collected
[34:43] Charge balance equation is out by -13.2%
[34:43] Stirrer speed set to 50
[34:48] pH 3.69 -> 3.49
[34:48] Using charge balance adjust
[34:48] Dispensed 0.000470 mL of Acid (0.5 M HCl)
[35:08] Stirrer speed set to 0
[35:18] Datapoint id 30 collected
[35:18] Charge balance equation is out by 6.0%
[35:18] Stirrer speed set to 50
[35:23] pH 3.48 -> 3.28
[35:23] Using charge balance adjust
[35:24] Dispensed 0.000776 mL of Acid (0.5 M HCl)
[35:44] Stirrer speed set to 0
[35:54] Datapoint id 31 collected
[35:54] Charge balance equation is out by 3.3%
[35:54] Stirrer speed set to 50
[35:59] pH 3.28 -> 3.08
[35:59] Using charge balance adjust
[35:59] Dispensed 0.001223 mL of Acid (0.5 M HCl)
[36:19] Stirrer speed set to 0
[36:29] Datapoint id 32 collected
[36:29] Charge balance equation is out by 2.2%
[36:29] Stirrer speed set to 50
[36:34] pH 3.08 -> 2.88
[36:34] Using charge balance adjust
[36:34] Dispensed 0.001929 mL of Acid (0.5 M HCl)
[36:55] Stirrer speed set to 0
[37:05] Datapoint id 33 collected
[37:05] Charge balance equation is out by 6.6%
[37:05] Stirrer speed set to 50
[37:10] pH 2.87 -> 2.67
[37:10] Using charge balance adjust
[37:10] Dispensed 0.003128 mL of Acid (0.5 M HCl)
[37:30] Stirrer speed set to 0
[37:40] Datapoint id 34 collected
[37:40] Charge balance equation is out by 9.6%
[37:40] Stirrer speed set to 50
[37:45] pH 2.66 -> 2.46
[37:45] Using charge balance adjust
[37:46] Dispensed 0.005151 mL of Acid (0.5 M HCl)
[38:06] Stirrer speed set to 0
[38:16] Datapoint id 35 collected
[38:16] Charge balance equation is out by 4.2%
[38:16] Stirrer speed set to 50
[38:21] pH 2.45 -> 2.25
[38:21] Using charge balance adjust
[38:21] Dispensed 0.008373 mL of Acid (0.5 M HCl)
[38:41] Stirrer speed set to 0
[38:52] Datapoint id 36 collected

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[38:52] Charge balance equation is out by -0.7%
[38:52] Stirrer speed set to 50
[38:57] pH 2.26 -> 2.06
[38:57] Using charge balance adjust
[38:57] Dispensed 0.013335 mL of Acid (0.5 M HCl)
[39:18] Stirrer speed set to 0
[39:28] Datapoint id 37 collected
[39:28] Charge balance equation is out by 6.9%
[39:28] Stirrer speed set to 50
[39:33] pH 2.05 -> 1.95
[39:33] Using charge balance adjust
[39:33] Dispensed 0.009737 mL of Acid (0.5 M HCl)
[39:54] Stirrer speed set to 0
[40:04] Datapoint id 38 collected
[40:04] Charge balance equation is out by -48.9%
[40:04] Titration 2 of 3
[40:04] Adding initial titrants
[40:04] Automatically add 0.20000 mL of Octanol
[40:08] Dispensed 0.200000 mL of Octanol
[40:08] Stirrer speed set to 10
[40:09] Stirrer speed set to 55
[40:09] Iterative adjust 1.95 -> 10.00
[40:09] pH 1.95 -> 10.00
[40:11] Dispensed 0.055880 mL of Base (0.5 M KOH)
[41:01] Stirrer speed set to 0
[41:48] Datapoint id 39 collected
[41:48] Stirrer speed set to 55
[41:53] pH 10.59 -> 10.39
[41:53] Using cautious pH adjust
[41:53] Dispensed 0.000329 mL of Acid (0.5 M HCl)
[41:58] Stepping pH = 10.50
[41:58] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[42:03] Stepping pH = 10.41
[42:03] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[42:08] Stepping pH = 10.40
[42:08] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[42:14] Stepping pH = 10.39
[42:29] Stirrer speed set to 0
[42:50] Datapoint id 40 collected
[42:50] Charge balance equation is out by -0.8%
[42:50] Stirrer speed set to 55
[42:55] pH 10.36 -> 10.16
[42:55] Using charge balance adjust
[42:55] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[43:15] Stirrer speed set to 0
[43:36] Datapoint id 41 collected
[43:36] Charge balance equation is out by 17.8%
[43:36] Stirrer speed set to 55
[43:41] pH 10.13 -> 9.93
[43:41] Using cautious pH adjust
[43:41] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[43:46] Stepping pH = 10.09
[43:46] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[43:51] Stepping pH = 9.88
[44:06] Stirrer speed set to 0
[44:16] Datapoint id 42 collected
[44:16] Charge balance equation is out by -46.0%
[44:16] Stirrer speed set to 55
[44:21] pH 9.86 -> 9.66

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[44:21] Using cautious pH adjust
[44:21] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[44:26] Stepping pH = 9.85
[44:27] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[44:32] Stepping pH = 9.55
[44:47] Stirrer speed set to 0
[45:05] Datapoint id 43 collected
[45:05] Charge balance equation is out by -94.9%
[45:05] Stirrer speed set to 55
[45:10] pH 9.51 -> 9.31
[45:10] Using cautious pH adjust
[45:10] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[45:15] Stepping pH = 9.50
[45:15] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[45:20] Stepping pH = 9.30
[45:36] Stirrer speed set to 0
[45:46] Datapoint id 44 collected
[45:46] Charge balance equation is out by -88.8%
[45:46] Stirrer speed set to 55
[45:51] pH 9.23 -> 9.03
[45:51] Using cautious pH adjust
[45:51] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[45:56] Stepping pH = 9.22
[45:56] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[46:01] Stepping pH = 9.10
[46:01] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[46:06] Stepping pH = 9.06
[46:06] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[46:11] Stepping pH = 9.02
[46:26] Stirrer speed set to 0
[46:38] Datapoint id 45 collected
[46:38] Charge balance equation is out by -183.9%
[46:38] Stirrer speed set to 55
[46:43] pH 8.90 -> 8.70
[46:43] Using cautious pH adjust
[46:44] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[46:49] Stepping pH = 8.89
[46:49] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[46:54] Stepping pH = 8.63
[47:09] Stirrer speed set to 0
[47:24] Datapoint id 46 collected
[47:24] Charge balance equation is out by -94.4%
[47:24] Stirrer speed set to 55
[47:29] pH 8.54 -> 8.34
[47:29] Using cautious pH adjust
[47:29] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[47:34] Stepping pH = 8.53
[47:34] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[47:39] Stepping pH = 8.30
[47:54] Stirrer speed set to 0
[48:10] Datapoint id 47 collected
[48:10] Charge balance equation is out by -96.0%
[48:10] Stirrer speed set to 55
[48:16] pH 8.23 -> 8.03
[48:16] Using cautious pH adjust
[48:16] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[48:21] Stepping pH = 8.20
[48:21] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[48:26] Stepping pH = 8.01

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:41] Stirrer speed set to 0
[48:55] Datapoint id 48 collected
[48:55] Charge balance equation is out by -69.2%
[48:55] Stirrer speed set to 55
[49:01] pH 7.95 -> 7.75
[49:01] Using cautious pH adjust
[49:01] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[49:06] Stepping pH = 7.87
[49:06] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[49:11] Stepping pH = 7.78
[49:11] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[49:16] Stepping pH = 7.75
[49:31] Stirrer speed set to 0
[49:45] Datapoint id 49 collected
[49:45] Charge balance equation is out by -25.6%
[49:45] Stirrer speed set to 55
[49:50] pH 7.72 -> 7.52
[49:50] Using cautious pH adjust
[49:50] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[49:55] Stepping pH = 7.62
[49:55] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[50:00] Stepping pH = 7.55
[50:00] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[50:05] Stepping pH = 7.53
[50:05] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[50:10] Stepping pH = 7.52
[50:25] Stirrer speed set to 0
[50:41] Datapoint id 50 collected
[50:41] Charge balance equation is out by -10.2%
[50:41] Stirrer speed set to 55
[50:46] pH 7.50 -> 7.30
[50:46] Using charge balance adjust
[50:46] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[51:06] Stirrer speed set to 0
[51:18] Datapoint id 51 collected
[51:18] Charge balance equation is out by -1.5%
[51:18] Stirrer speed set to 55
[51:23] pH 7.29 -> 7.09
[51:23] Using charge balance adjust
[51:23] Dispensed 0.000611 mL of Acid (0.5 M HCl)
[51:43] Stirrer speed set to 0
[51:55] Datapoint id 52 collected
[51:55] Charge balance equation is out by -3.4%
[51:55] Stirrer speed set to 55
[52:00] pH 7.09 -> 6.89
[52:00] Using charge balance adjust
[52:01] Dispensed 0.000776 mL of Acid (0.5 M HCl)
[52:21] Stirrer speed set to 0
[52:33] Datapoint id 53 collected
[52:33] Charge balance equation is out by -3.7%
[52:33] Stirrer speed set to 55
[52:38] pH 6.89 -> 6.69
[52:38] Using charge balance adjust
[52:38] Dispensed 0.000941 mL of Acid (0.5 M HCl)
[52:59] Stirrer speed set to 0
[53:11] Datapoint id 54 collected
[53:11] Charge balance equation is out by 3.2%
[53:11] Stirrer speed set to 55
[53:16] pH 6.69 -> 6.49

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[53:16] Using charge balance adjust
[53:16] Dispensed 0.001011 mL of Acid (0.5 M HCl)
[53:37] Stirrer speed set to 0
[53:51] Datapoint id 55 collected
[53:51] Charge balance equation is out by 1.7%
[53:51] Stirrer speed set to 55
[53:56] pH 6.48 -> 6.28
[53:56] Using charge balance adjust
[53:56] Dispensed 0.000988 mL of Acid (0.5 M HCl)
[54:17] Stirrer speed set to 0
[54:33] Datapoint id 56 collected
[54:33] Charge balance equation is out by 3.6%
[54:33] Stirrer speed set to 55
[54:38] pH 6.26 -> 6.06
[54:38] Using charge balance adjust
[54:38] Dispensed 0.000847 mL of Acid (0.5 M HCl)
[54:58] Stirrer speed set to 0
[55:14] Datapoint id 57 collected
[55:14] Charge balance equation is out by 4.4%
[55:14] Stirrer speed set to 55
[55:19] pH 6.04 -> 5.84
[55:19] Using charge balance adjust
[55:19] Dispensed 0.000682 mL of Acid (0.5 M HCl)
[55:39] Stirrer speed set to 0
[55:54] Datapoint id 58 collected
[55:54] Charge balance equation is out by 4.2%
[55:54] Stirrer speed set to 55
[55:59] pH 5.82 -> 5.62
[55:59] Using charge balance adjust
[55:59] Dispensed 0.000470 mL of Acid (0.5 M HCl)
[56:19] Stirrer speed set to 0
[56:34] Datapoint id 59 collected
[56:34] Charge balance equation is out by -5.4%
[56:34] Stirrer speed set to 55
[56:39] pH 5.61 -> 5.41
[56:39] Using charge balance adjust
[56:39] Dispensed 0.000329 mL of Acid (0.5 M HCl)
[56:59] Stirrer speed set to 0
[57:14] Datapoint id 60 collected
[57:14] Charge balance equation is out by -8.3%
[57:14] Stirrer speed set to 55
[57:19] pH 5.41 -> 5.21
[57:19] Using charge balance adjust
[57:19] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[57:39] Stirrer speed set to 0
[57:54] Datapoint id 61 collected
[57:54] Charge balance equation is out by -7.7%
[57:54] Stirrer speed set to 55
[57:59] pH 5.20 -> 5.00
[57:59] Using charge balance adjust
[57:59] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[58:19] Stirrer speed set to 0
[58:33] Datapoint id 62 collected
[58:33] Charge balance equation is out by -25.6%
[58:33] Stirrer speed set to 55
[58:38] pH 5.02 -> 4.82
[58:38] Using cautious pH adjust
[58:38] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[58:44] Stepping pH = 4.97

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[58:44] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[58:49] Stepping pH = 4.80
[59:04] Stirrer speed set to 0
[59:17] Datapoint id 63 collected
[59:17] Charge balance equation is out by -23.5%
[59:17] Stirrer speed set to 55
[59:22] pH 4.77 -> 4.57
[59:22] Using cautious pH adjust
[59:22] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[59:27] Stepping pH = 4.74
[59:27] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[59:32] Stepping pH = 4.49
[59:47] Stirrer speed set to 0
[1:00:01] Datapoint id 64 collected
[1:00:01] Charge balance equation is out by -69.6%
[1:00:01] Stirrer speed set to 55
[1:00:06] pH 4.47 -> 4.27
[1:00:06] Using cautious pH adjust
[1:00:06] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:00:11] Stepping pH = 4.45
[1:00:11] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:00:16] Stepping pH = 4.20
[1:00:31] Stirrer speed set to 0
[1:00:43] Datapoint id 65 collected
[1:00:43] Charge balance equation is out by -85.9%
[1:00:43] Stirrer speed set to 55
[1:00:48] pH 4.19 -> 3.99
[1:00:48] Using cautious pH adjust
[1:00:48] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:00:53] Stepping pH = 4.10
[1:00:53] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:00:58] Stepping pH = 4.03
[1:00:58] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:01:04] Stepping pH = 4.00
[1:01:04] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:01:09] Stepping pH = 3.98
[1:01:24] Stirrer speed set to 0
[1:01:34] Datapoint id 66 collected
[1:01:34] Charge balance equation is out by -32.8%
[1:01:34] Stirrer speed set to 55
[1:01:39] pH 3.97 -> 3.77
[1:01:39] Using cautious pH adjust
[1:01:39] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:01:44] Stepping pH = 3.87
[1:01:44] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:01:49] Stepping pH = 3.81
[1:01:49] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:01:54] Stepping pH = 3.78
[1:01:54] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:01:59] Stepping pH = 3.78
[1:02:14] Stirrer speed set to 0
[1:02:25] Datapoint id 67 collected
[1:02:25] Charge balance equation is out by -15.5%
[1:02:25] Stirrer speed set to 55
[1:02:30] pH 3.77 -> 3.57
[1:02:30] Using cautious pH adjust
[1:02:30] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[1:02:35] Stepping pH = 3.66
[1:02:35] Dispensed 0.000141 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:02:40] Stepping pH = 3.61
[1:02:41] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:02:46] Stepping pH = 3.58
[1:03:01] Stirrer speed set to 0
[1:03:11] Datapoint id 68 collected
[1:03:11] Charge balance equation is out by -6.3%
[1:03:11] Stirrer speed set to 55
[1:03:16] pH 3.57 -> 3.37
[1:03:16] Using charge balance adjust
[1:03:16] Dispensed 0.000659 mL of Acid (0.5 M HCl)
[1:03:36] Stirrer speed set to 0
[1:03:46] Datapoint id 69 collected
[1:03:46] Charge balance equation is out by -2.7%
[1:03:46] Stirrer speed set to 55
[1:03:51] pH 3.37 -> 3.17
[1:03:51] Using charge balance adjust
[1:03:51] Dispensed 0.001035 mL of Acid (0.5 M HCl)
[1:04:12] Stirrer speed set to 0
[1:04:22] Datapoint id 70 collected
[1:04:22] Charge balance equation is out by -8.0%
[1:04:22] Stirrer speed set to 55
[1:04:27] pH 3.19 -> 2.99
[1:04:27] Using charge balance adjust
[1:04:27] Dispensed 0.001576 mL of Acid (0.5 M HCl)
[1:04:47] Stirrer speed set to 0
[1:04:57] Datapoint id 71 collected
[1:04:57] Charge balance equation is out by -5.6%
[1:04:57] Stirrer speed set to 55
[1:05:02] pH 3.01 -> 2.81
[1:05:02] Using charge balance adjust
[1:05:02] Dispensed 0.002446 mL of Acid (0.5 M HCl)
[1:05:23] Stirrer speed set to 0
[1:05:33] Datapoint id 72 collected
[1:05:33] Charge balance equation is out by -1.4%
[1:05:33] Stirrer speed set to 55
[1:05:38] pH 2.81 -> 2.61
[1:05:38] Using charge balance adjust
[1:05:38] Dispensed 0.003833 mL of Acid (0.5 M HCl)
[1:05:58] Stirrer speed set to 0
[1:06:08] Datapoint id 73 collected
[1:06:08] Charge balance equation is out by -0.1%
[1:06:08] Stirrer speed set to 55
[1:06:13] pH 2.61 -> 2.41
[1:06:13] Using charge balance adjust
[1:06:13] Dispensed 0.006115 mL of Acid (0.5 M HCl)
[1:06:34] Stirrer speed set to 0
[1:06:44] Datapoint id 74 collected
[1:06:44] Charge balance equation is out by 5.7%
[1:06:44] Stirrer speed set to 55
[1:06:49] pH 2.41 -> 2.21
[1:06:49] Using charge balance adjust
[1:06:50] Dispensed 0.010042 mL of Acid (0.5 M HCl)
[1:07:10] Stirrer speed set to 0
[1:07:20] Datapoint id 75 collected
[1:07:20] Charge balance equation is out by -0.1%
[1:07:20] Stirrer speed set to 55
[1:07:25] pH 2.21 -> 2.01
[1:07:25] Using charge balance adjust
[1:07:26] Dispensed 0.016181 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:07:46] Stirrer speed set to 0
[1:07:56] Datapoint id 76 collected
[1:07:56] Charge balance equation is out by 1.9%
[1:07:56] Stirrer speed set to 55
[1:08:01] pH 2.01 -> 1.95
[1:08:01] Using charge balance adjust
[1:08:02] Dispensed 0.006491 mL of Acid (0.5 M HCl)
[1:08:22] Stirrer speed set to 0
[1:08:32] Datapoint id 77 collected
[1:08:32] Charge balance equation is out by -70.0%
[1:08:32] Titration 3 of 3
[1:08:32] Adding initial titrants
[1:08:32] Automatically add 0.80000 mL of Octanol
[1:09:23] Dispensed 0.800000 mL of Octanol
[1:09:23] Stirrer speed set to 10
[1:09:24] Stirrer speed set to 60
[1:09:24] Iterative adjust 1.95 -> 10.00
[1:09:24] pH 1.95 -> 10.00
[1:09:25] Dispensed 0.059925 mL of Base (0.5 M KOH)
[1:10:15] Stirrer speed set to 0
[1:10:34] Datapoint id 78 collected
[1:10:34] Stirrer speed set to 60
[1:10:40] pH 10.30 -> 10.10
[1:10:40] Using cautious pH adjust
[1:10:40] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[1:10:45] Stepping pH = 10.28
[1:10:45] Dispensed 0.000541 mL of Acid (0.5 M HCl)
[1:10:50] Stepping pH = 9.94
[1:11:05] Stirrer speed set to 0
[1:11:34] Datapoint id 79 collected
[1:11:34] Charge balance equation is out by -81.9%
[1:11:34] Stirrer speed set to 60
[1:11:39] pH 9.90 -> 9.70
[1:11:39] Using cautious pH adjust
[1:11:39] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:11:44] Stepping pH = 9.90
[1:11:44] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[1:11:50] Stepping pH = 9.63
[1:12:05] Stirrer speed set to 0
[1:12:15] Datapoint id 80 collected
[1:12:15] Charge balance equation is out by -91.9%
[1:12:15] Stirrer speed set to 60
[1:12:20] pH 9.60 -> 9.40
[1:12:20] Using cautious pH adjust
[1:12:20] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:12:25] Stepping pH = 9.60
[1:12:25] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:12:30] Stepping pH = 9.43
[1:12:30] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:12:35] Stepping pH = 9.42
[1:12:35] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:12:40] Stepping pH = 9.40
[1:12:55] Stirrer speed set to 0
[1:13:05] Datapoint id 81 collected
[1:13:05] Charge balance equation is out by -132.7%
[1:13:05] Stirrer speed set to 60
[1:13:11] pH 9.37 -> 9.17
[1:13:11] Using cautious pH adjust
[1:13:11] Dispensed 0.000047 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:13:16] Stepping pH = 9.36
[1:13:16] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:13:21] Stepping pH = 9.14
[1:13:36] Stirrer speed set to 0
[1:13:47] Datapoint id 82 collected
[1:13:47] Charge balance equation is out by -88.9%
[1:13:47] Stirrer speed set to 60
[1:13:53] pH 9.10 -> 8.90
[1:13:53] Using cautious pH adjust
[1:13:53] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:13:58] Stepping pH = 9.08
[1:13:58] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:14:03] Stepping pH = 8.86
[1:14:18] Stirrer speed set to 0
[1:14:33] Datapoint id 83 collected
[1:14:33] Charge balance equation is out by -89.5%
[1:14:33] Stirrer speed set to 60
[1:14:38] pH 8.81 -> 8.61
[1:14:38] Using cautious pH adjust
[1:14:38] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:14:43] Stepping pH = 8.80
[1:14:43] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:14:48] Stepping pH = 8.51
[1:15:04] Stirrer speed set to 0
[1:15:26] Datapoint id 84 collected
[1:15:26] Charge balance equation is out by -94.1%
[1:15:26] Stirrer speed set to 60
[1:15:31] pH 8.48 -> 8.28
[1:15:31] Using cautious pH adjust
[1:15:31] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:15:36] Stepping pH = 8.44
[1:15:36] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[1:15:41] Stepping pH = 8.22
[1:15:56] Stirrer speed set to 0
[1:16:20] Datapoint id 85 collected
[1:16:20] Charge balance equation is out by -44.0%
[1:16:20] Stirrer speed set to 60
[1:16:25] pH 8.19 -> 7.99
[1:16:25] Using cautious pH adjust
[1:16:25] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:16:30] Stepping pH = 8.11
[1:16:30] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:16:35] Stepping pH = 8.01
[1:16:35] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:16:40] Stepping pH = 8.00
[1:16:40] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:16:45] Stepping pH = 7.99
[1:17:00] Stirrer speed set to 0
[1:17:23] Datapoint id 86 collected
[1:17:23] Charge balance equation is out by -19.6%
[1:17:23] Stirrer speed set to 60
[1:17:28] pH 7.97 -> 7.77
[1:17:28] Using cautious pH adjust
[1:17:28] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[1:17:33] Stepping pH = 7.85
[1:17:33] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:17:38] Stepping pH = 7.79
[1:17:38] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:17:43] Stepping pH = 7.79

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:17:43] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:17:48] Stepping pH = 7.78
[1:18:03] Stirrer speed set to 0
[1:18:26] Datapoint id 87 collected
[1:18:26] Charge balance equation is out by 3.4%
[1:18:26] Stirrer speed set to 60
[1:18:31] pH 7.76 -> 7.56
[1:18:31] Using charge balance adjust
[1:18:31] Dispensed 0.000659 mL of Acid (0.5 M HCl)
[1:18:51] Stirrer speed set to 0
[1:19:12] Datapoint id 88 collected
[1:19:12] Charge balance equation is out by 13.2%
[1:19:12] Stirrer speed set to 60
[1:19:17] pH 7.52 -> 7.32
[1:19:17] Using charge balance adjust
[1:19:17] Dispensed 0.000870 mL of Acid (0.5 M HCl)
[1:19:37] Stirrer speed set to 0
[1:20:00] Datapoint id 89 collected
[1:20:00] Charge balance equation is out by 2.1%
[1:20:00] Stirrer speed set to 60
[1:20:05] pH 7.30 -> 7.10
[1:20:05] Using charge balance adjust
[1:20:05] Dispensed 0.000988 mL of Acid (0.5 M HCl)
[1:20:26] Stirrer speed set to 0
[1:20:50] Datapoint id 90 collected
[1:20:50] Charge balance equation is out by -5.8%
[1:20:50] Stirrer speed set to 60
[1:20:55] pH 7.09 -> 6.89
[1:20:55] Using charge balance adjust
[1:20:55] Dispensed 0.001011 mL of Acid (0.5 M HCl)
[1:21:15] Stirrer speed set to 0
[1:21:38] Datapoint id 91 collected
[1:21:38] Charge balance equation is out by -9.0%
[1:21:38] Stirrer speed set to 60
[1:21:43] pH 6.88 -> 6.68
[1:21:43] Using charge balance adjust
[1:21:43] Dispensed 0.000917 mL of Acid (0.5 M HCl)
[1:22:04] Stirrer speed set to 0
[1:22:33] Datapoint id 92 collected
[1:22:33] Charge balance equation is out by -16.1%
[1:22:33] Stirrer speed set to 60
[1:22:38] pH 6.67 -> 6.47
[1:22:38] Using cautious pH adjust
[1:22:38] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[1:22:43] Stepping pH = 6.57
[1:22:43] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[1:22:48] Stepping pH = 6.50
[1:22:48] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:22:53] Stepping pH = 6.48
[1:22:53] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:22:58] Stepping pH = 6.47
[1:23:13] Stirrer speed set to 0
[1:23:43] Datapoint id 93 collected
[1:23:43] Charge balance equation is out by -7.8%
[1:23:43] Stirrer speed set to 60
[1:23:48] pH 6.47 -> 6.27
[1:23:48] Using charge balance adjust
[1:23:48] Dispensed 0.000564 mL of Acid (0.5 M HCl)
[1:24:08] Stirrer speed set to 0

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:24:40] Datapoint id 94 collected
[1:24:40] Charge balance equation is out by -25.7%
[1:24:40] Stirrer speed set to 60
[1:24:45] pH 6.26 -> 6.06
[1:24:45] Using cautious pH adjust
[1:24:45] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[1:24:50] Stepping pH = 6.18
[1:24:50] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:24:55] Stepping pH = 6.10
[1:24:55] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:25:01] Stepping pH = 6.07
[1:25:16] Stirrer speed set to 0
[1:25:47] Datapoint id 95 collected
[1:25:47] Charge balance equation is out by -6.6%
[1:25:47] Stirrer speed set to 60
[1:25:52] pH 6.08 -> 5.88
[1:25:52] Using charge balance adjust
[1:25:52] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[1:26:13] Stirrer speed set to 0
[1:26:32] Datapoint id 96 collected
[1:26:32] Charge balance equation is out by -37.9%
[1:26:32] Stirrer speed set to 60
[1:26:37] pH 5.89 -> 5.69
[1:26:37] Using cautious pH adjust
[1:26:37] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:26:42] Stepping pH = 5.84
[1:26:42] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:26:47] Stepping pH = 5.71
[1:26:47] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:26:52] Stepping pH = 5.70
[1:27:07] Stirrer speed set to 0
[1:27:26] Datapoint id 97 collected
[1:27:26] Charge balance equation is out by -33.9%
[1:27:26] Stirrer speed set to 60
[1:27:31] pH 5.69 -> 5.49
[1:27:31] Using cautious pH adjust
[1:27:31] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:27:36] Stepping pH = 5.64
[1:27:36] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:27:41] Stepping pH = 5.45
[1:27:56] Stirrer speed set to 0
[1:28:14] Datapoint id 98 collected
[1:28:14] Charge balance equation is out by -30.0%
[1:28:14] Stirrer speed set to 60
[1:28:19] pH 5.45 -> 5.25
[1:28:19] Using cautious pH adjust
[1:28:19] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:28:24] Stepping pH = 5.42
[1:28:24] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:28:29] Stepping pH = 5.22
[1:28:44] Stirrer speed set to 0
[1:29:01] Datapoint id 99 collected
[1:29:01] Charge balance equation is out by -55.8%
[1:29:01] Stirrer speed set to 60
[1:29:07] pH 5.20 -> 5.00
[1:29:07] Using cautious pH adjust
[1:29:07] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:29:12] Stepping pH = 5.19
[1:29:12] Dispensed 0.000094 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:29:17] Stepping pH = 4.93
[1:29:32] Stirrer speed set to 0
[1:29:54] Datapoint id 100 collected
[1:29:54] Charge balance equation is out by -94.2%
[1:29:54] Stirrer speed set to 60
[1:29:59] pH 4.89 -> 4.69
[1:29:59] Using cautious pH adjust
[1:29:59] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:30:04] Stepping pH = 4.89
[1:30:04] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:30:09] Stepping pH = 4.71
[1:30:09] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:30:14] Stepping pH = 4.65
[1:30:30] Stirrer speed set to 0
[1:30:47] Datapoint id 101 collected
[1:30:47] Charge balance equation is out by -132.2%
[1:30:47] Stirrer speed set to 60
[1:30:52] pH 4.63 -> 4.43
[1:30:52] Using cautious pH adjust
[1:30:52] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:30:57] Stepping pH = 4.56
[1:30:57] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:31:03] Stepping pH = 4.46
[1:31:03] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:31:08] Stepping pH = 4.42
[1:31:23] Stirrer speed set to 0
[1:31:34] Datapoint id 102 collected
[1:31:34] Charge balance equation is out by -38.2%
[1:31:34] Stirrer speed set to 60
[1:31:39] pH 4.41 -> 4.21
[1:31:39] Using cautious pH adjust
[1:31:39] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:31:44] Stepping pH = 4.38
[1:31:44] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:31:49] Stepping pH = 4.16
[1:32:04] Stirrer speed set to 0
[1:32:14] Datapoint id 103 collected
[1:32:14] Charge balance equation is out by -54.7%
[1:32:14] Stirrer speed set to 60
[1:32:19] pH 4.15 -> 3.95
[1:32:19] Using cautious pH adjust
[1:32:20] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:32:25] Stepping pH = 4.07
[1:32:25] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:32:30] Stepping pH = 3.98
[1:32:30] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:32:35] Stepping pH = 3.96
[1:32:50] Stirrer speed set to 0
[1:33:00] Datapoint id 104 collected
[1:33:00] Charge balance equation is out by -11.2%
[1:33:00] Stirrer speed set to 60
[1:33:05] pH 3.95 -> 3.75
[1:33:05] Using charge balance adjust
[1:33:05] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[1:33:25] Stirrer speed set to 0
[1:33:44] Datapoint id 105 collected
[1:33:44] Charge balance equation is out by 5.1%
[1:33:44] Stirrer speed set to 60
[1:33:49] pH 3.74 -> 3.54

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02007**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 5:10:52 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:33:49] Using charge balance adjust
[1:33:49] Dispensed 0.000470 mL of Acid (0.5 M HCl)
[1:34:09] Stirrer speed set to 0
[1:34:19] Datapoint id 106 collected
[1:34:19] Charge balance equation is out by -1.6%
[1:34:19] Stirrer speed set to 60
[1:34:24] pH 3.54 -> 3.34
[1:34:24] Using charge balance adjust
[1:34:25] Dispensed 0.000753 mL of Acid (0.5 M HCl)
[1:34:45] Stirrer speed set to 0
[1:34:55] Datapoint id 107 collected
[1:34:55] Charge balance equation is out by 2.6%
[1:34:55] Stirrer speed set to 60
[1:35:00] pH 3.34 -> 3.14
[1:35:00] Using charge balance adjust
[1:35:00] Dispensed 0.001199 mL of Acid (0.5 M HCl)
[1:35:20] Stirrer speed set to 0
[1:35:30] Datapoint id 108 collected
[1:35:30] Charge balance equation is out by 2.0%
[1:35:30] Stirrer speed set to 60
[1:35:35] pH 3.14 -> 2.94
[1:35:35] Using charge balance adjust
[1:35:36] Dispensed 0.001905 mL of Acid (0.5 M HCl)
[1:35:56] Stirrer speed set to 0
[1:36:06] Datapoint id 109 collected
[1:36:06] Charge balance equation is out by -1.1%
[1:36:06] Stirrer speed set to 60
[1:36:11] pH 2.95 -> 2.75
[1:36:11] Using charge balance adjust
[1:36:11] Dispensed 0.002987 mL of Acid (0.5 M HCl)
[1:36:31] Stirrer speed set to 0
[1:36:56] Datapoint id 110 collected
[1:36:56] Charge balance equation is out by -5.0%
[1:36:56] Stirrer speed set to 60
[1:37:01] pH 2.76 -> 2.56
[1:37:01] Using charge balance adjust
[1:37:01] Dispensed 0.004610 mL of Acid (0.5 M HCl)
[1:37:21] Stirrer speed set to 0
[1:37:47] Datapoint id 111 collected
[1:37:47] Charge balance equation is out by -2.3%
[1:37:47] Stirrer speed set to 60
[1:37:52] pH 2.57 -> 2.37
[1:37:52] Using charge balance adjust
[1:37:52] Dispensed 0.007244 mL of Acid (0.5 M HCl)
[1:38:13] Stirrer speed set to 0
[1:38:25] Datapoint id 112 collected
[1:38:25] Charge balance equation is out by 1.1%
[1:38:25] Stirrer speed set to 60
[1:38:30] pH 2.38 -> 2.18
[1:38:30] Using charge balance adjust
[1:38:30] Dispensed 0.011571 mL of Acid (0.5 M HCl)
[1:38:50] Stirrer speed set to 0
[1:39:06] Datapoint id 113 collected
[1:39:06] Charge balance equation is out by -0.0%
[1:39:06] Stirrer speed set to 60
[1:39:11] pH 2.18 -> 1.98
[1:39:11] Using charge balance adjust
[1:39:11] Dispensed 0.018650 mL of Acid (0.5 M HCl)
[1:39:32] Stirrer speed set to 0

Sample name:	**M08_octanol**	Experiment start time:	**3/2/2018 5:10:52 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18C-02007**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02007_M08_octanol_pH-metric high logP.t3r**		

Experiment Log (continued)

[1:39:43] Datapoint id 114 collected
[1:39:43] Charge balance equation is out by 0.2%
[1:39:43] Argon flow rate set to 0
[1:39:47] Titrator arm moved over Titration position